

9,10-ANTHRACENEDIONE

Other names:	9,10(9H,10H)-anthracenedione
	9,10-Anthrachinon
	9,10-anthracenequinone
	9,10-anthraquinone
	9,10-dioxoanthracene
	Anthracene, 9,10-dihydro-9,10-dioxo-
	Anthracene-9,10-quinone
	Anthradione
	Corbit
	Hoelite
	Morkit
	NSC 7957
	anthracene-9,10-dione
	anthraquinone
Inchi:	InChI=1S/C14H8O2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H
InchiKey:	RZVHIXYEVGDQDX-UHFFFAOYSA-N
Formula:	C14H8O2
SMILES:	O=C1c2ccccc2C(=O)c2ccccc21
Mol. weight [g/mol]:	208.22
CAS:	84-65-1

Physical Properties

Property code	Value	Unit	Source
af	0.5927		Cheméo Relay (1.0)
chs	-6444.52	kJ/mol	NIST Webbook
chs	-6462.20	kJ/mol	NIST Webbook
chs	-6468.90	kJ/mol	NIST Webbook
chs	-6464.00 ± 2.10	kJ/mol	NIST Webbook
ea	1.59 ± 0.06	eV	NIST Webbook
ea	1.15 ± 0.10	eV	NIST Webbook
hf	-75.70 ± 2.90	kJ/mol	NIST Webbook
hfs	-188.50 ± 2.80	kJ/mol	NIST Webbook
hfus	36.30	kJ/mol	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
hsub	112.00	kJ/mol	NIST Webbook
hsub	137.00 ± 3.00	kJ/mol	NIST Webbook

hsub	107.90	kJ/mol	NIST Webbook
hsub	110.90	kJ/mol	NIST Webbook
hsub	112.80	kJ/mol	NIST Webbook
hsub	108.00	kJ/mol	NIST Webbook
hsub	113.00 ± 0.80	kJ/mol	NIST Webbook
hsub	112.10	kJ/mol	NIST Webbook
hvap	94.56	kJ/mol	Cheméo Relay (1.0)
ie	9.25 ± 0.12	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.25 ± 0.03	eV	NIST Webbook
ie	9.40 ± 0.08	eV	NIST Webbook
log10ws	-5.19		Estimated Solubility Method
log10ws	-5.19		Aqueous Solubility Prediction Method
logp	2.462		Crippen Method
mcvol	152.880	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	330.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	331.09		NIST Webbook
rinpol	329.60		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	331.32		NIST Webbook
rinpol	331.91		NIST Webbook
rinpol	333.00		NIST Webbook
rinpol	329.00		NIST Webbook
rinpol	330.90		NIST Webbook
rinpol	337.40		NIST Webbook
rinpol	331.22		NIST Webbook
rinpol	331.09		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	331.38		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	331.22		NIST Webbook
rinpol	330.26		NIST Webbook
rinpol	330.50		NIST Webbook
rinpol	330.70		NIST Webbook
tb	653.20	K	NIST Webbook
tb	650.00 ± 0.30	K	NIST Webbook

tb	650.00 ± 0.30	K	NIST Webbook
tc	933.95	K	Cheméo Relay (1.0)
tf	557.78 ± 0.30	K	NIST Webbook
tf	557.85 ± 0.20	K	NIST Webbook
tf	555.00 ± 1.00	K	NIST Webbook
tf	558.35 ± 0.40	K	NIST Webbook
tf	558.15 ± 1.00	K	NIST Webbook
tf	557.96 ± 0.20	K	NIST Webbook
tf	558.07 ± 0.20	K	NIST Webbook
tf	557.75 ± 0.30	K	NIST Webbook
tf	557.97 ± 0.35	K	NIST Webbook
tf	557.75 ± 0.50	K	NIST Webbook
vc	0.570	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.41	J/mol×K	817.56	Joback Method
cpg	415.60	J/mol×K	771.69	Joback Method
cpg	468.21	J/mol×K	1001.05	Joback Method
cpg	401.54	J/mol×K	725.82	Joback Method
cpg	459.88	J/mol×K	955.18	Joback Method
cpg	450.50	J/mol×K	909.31	Joback Method
cpg	440.03	J/mol×K	863.44	Joback Method
cps	240.20	J/mol×K	298.15	NIST Webbook
hfust	32.57	kJ/mol	555.00	NIST Webbook
hfust	32.57	kJ/mol	555.00	NIST Webbook
hfust	32.57	kJ/mol	558.00	NIST Webbook
hsubt	126.40	kJ/mol	373.00	NIST Webbook
hsubt	127.00 ± 3.00	kJ/mol	530.00	NIST Webbook
hsubt	107.90 ± 0.80	kJ/mol	434.00	NIST Webbook
hsubt	107.50 ± 0.80	kJ/mol	434.00	NIST Webbook
hsubt	98.30	kJ/mol	413.00	NIST Webbook
hsubt	104.60	kJ/mol	367.00	NIST Webbook
hvapt	64.30	kJ/mol	609.50	NIST Webbook

psub	2.63e-04	kPa	385.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	0.02	kPa	429.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	4.10e-05	kPa	367.40	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	5.42e-05	kPa	369.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.19e-04	kPa	377.60	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.44e-04	kPa	379.20	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	1.49e-04	kPa	380.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	2.67e-04	kPa	385.40	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	2.20e-05	kPa	360.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	3.05e-04	kPa	386.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	4.93e-04	kPa	392.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	4.94e-04	kPa	392.80	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	5.19e-04	kPa	393.40	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	8.72e-04	kPa	399.20	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	9.48e-04	kPa	399.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	0.01	kPa	422.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.02	kPa	427.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	2.52e-05	kPa	362.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	0.02	kPa	432.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.03	kPa	437.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.04	kPa	439.10	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.04	kPa	441.60	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.05	kPa	447.20	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.07	kPa	448.90	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.08	kPa	451.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.10	kPa	457.00	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.15	kPa	458.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.17	kPa	460.40	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.20	kPa	466.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.27	kPa	468.70	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.25	kPa	469.80	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds

psub	0.32	kPa	476.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	0.49	kPa	478.50	Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds
psub	2.09e-05	kPa	359.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	4.49e-06	kPa	346.00	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
sfust	58.70	J/mol×K	555.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.75139e+01
Coeff. B	-8.78545e+03
Coeff. C	2.80780e+01
Temperature range (K), min.	481.92
Temperature range (K), max.	691.90

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure: Cheméo Relay (1.0, beta):	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Cheméo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured by the Knudsen effusion technique:	https://www.doi.org/10.1016/j.jct.2010.01.014
Sublimation/vaporization enthalpy at 106.3 K	https://www.doi.org/10.1016/j.tca.2016.03.031
Sublimation of Anthracene-Like Compounds	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1216
Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water:	https://www.doi.org/10.1021/je100850z
Aqueous Solubility Prediction Method:	https://www.doi.org/10.1021/je800707x
McGowan Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Fast scanning calorimetry: Sublimation thermodynamics of low volatile and thermally unstable compounds:	http://link.springer.com/article/10.1007/BF02311772
	https://www.doi.org/10.1016/j.tca.2019.05.008
	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84651&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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