

Anthrone

Other names:	(10H)-9-Anthracenone 9(10H)-anthracenone 9,10-Dihydro-9-oxoanthracene 9,10-dihydro-9-anthracenone Anthracene, 9,10-dihydro-9-oxo- Carbothrone
Inchi:	InChI=1S/C14H10O/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-8H,9H2
InchiKey:	RJGDLRCDCYRQOQ-UHFFFAOYSA-N
Formula:	C14H10O
SMILES:	O=C1c2ccccc2Cc2ccccc21
Mol. weight [g/mol]:	194.23
CAS:	90-44-8

Physical Properties

Property code	Value	Unit	Source
chs	-6858.40 ± 1.90	kJ/mol	NIST Webbook
gf	230.53	kJ/mol	Joback Method
hf	23.40 ± 2.20	kJ/mol	NIST Webbook
hfs	-79.90 ± 2.10	kJ/mol	NIST Webbook
hfus	22.40	kJ/mol	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
hsub	103.32 ± 0.63	kJ/mol	NIST Webbook
hsub	103.30	kJ/mol	NIST Webbook
hsub	106.10 ± 0.80	kJ/mol	NIST Webbook
hsub	103.30	kJ/mol	NIST Webbook
hvap	56.93	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook
ie	9.43	eV	NIST Webbook
ie	8.83 ± 0.03	eV	NIST Webbook
ie	8.83 ± 0.03	eV	NIST Webbook
log10ws	-3.78		Crippen Method
logp	2.822		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	298.40		NIST Webbook

rinpol	1904.00		NIST Webbook
rinpol	331.39		NIST Webbook
rinpol	298.40		NIST Webbook
rinpol	332.60		NIST Webbook
rinpol	330.10		NIST Webbook
rinpol	330.53		NIST Webbook
rinpol	331.39		NIST Webbook
rinpol	330.53		NIST Webbook
rinpol	331.00		NIST Webbook
rinpol	328.09		NIST Webbook
rinpol	297.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	330.10		NIST Webbook
tb	658.00	K	Joback Method
tc	922.12	K	Joback Method
tf	428.15 ± 3.00	K	NIST Webbook
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.22	J/mol×K	658.00	Joback Method
cpg	443.22	J/mol×K	878.10	Joback Method
cpg	432.50	J/mol×K	834.08	Joback Method
cpg	420.84	J/mol×K	790.06	Joback Method
cpg	408.14	J/mol×K	746.04	Joback Method
cpg	394.30	J/mol×K	702.02	Joback Method
cpg	453.12	J/mol×K	922.12	Joback Method
hfust	26.80	kJ/mol	429.00	NIST Webbook
hfust	26.80	kJ/mol	429.00	NIST Webbook
hfust	26.80	kJ/mol	429.00	NIST Webbook
hsubt	99.60	kJ/mol	354.00	NIST Webbook
hsubt	1037.30	kJ/mol	298.15	NIST Webbook
hvapt	106.70	kJ/mol	298.15	Energetic effects of ether and ketone functional groups in 9,10-dihydroanthracene compound

Sources

Solubilities of Oxygenated Aromatic Solids in Pressurized Hot Water: Joback Method:

<https://www.doi.org/10.1021/je800707x>

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C90448&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Energetic effects of ether and ketone functional groups in

https://www.chemeo.com/doc/models/crippen_log10ws

the dynamic study on the Sublimation of Anthracene-Like Compounds:

<https://www.doi.org/10.1016/j.jct.2010.04.027>

<https://www.doi.org/10.1021/je100850z>

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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