

7H-Benz[de]anthracen-7-one

Other names:	1,9-benz-10-anthrone
	7-oxobenz[de]anthracene
	7H-Benz[de]anthracene-7-one
	7H-Benzo(de)anthracen-7-one
	Benzanthrone
	Benzoanthrone
	Dye, benzanthrone
	Ms-Benzanthrone
	NSC 5189
	NSC 631641
	benz[de]anthracen-7-one
	benzanthrenone
	benzanthrone
	naphthanthrone
Inchi:	InChI=1S/C17H10O/c18-17-14-8-2-1-7-12(14)13-9-3-5-11-6-4-10-15(17)16(11)13/h1-10H
InchiKey:	HUKPVYBUJRAUAG-UHFFFAOYSA-N
Formula:	C17H10O
SMILES:	O=C1c2ccccc2-c2cccc3cccc1c23
Mol. weight [g/mol]:	230.26
CAS:	82-05-3

Physical Properties

Property code	Value	Unit	Source
gf	364.91	kJ/mol	Joback Method
hf	203.27	kJ/mol	Joback Method
hfus	125.40	kJ/mol	New Knudsen effusion apparatus with simultaneous gravimetric and quartz crystal microbalance mass loss detection
hfus	125.40	kJ/mol	New Knudsen effusion apparatus with simultaneous gravimetric and quartz crystal microbalance mass loss detection

hfus	125.30	kJ/mol	New Knudsen effusion apparatus with simultaneous gravimetric and quartz crystal microbalance mass loss detection
hsub	124.60 ± 6.00	kJ/mol	NIST Webbook
hsub	129.70 ± 2.10	kJ/mol	NIST Webbook
hsub	126.60 ± 0.60	kJ/mol	NIST Webbook
hsub	125.60 ± 0.60	kJ/mol	NIST Webbook
hvap	65.74	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-6.08		Crippen Method
logp	4.051		Crippen Method
mcvol	174.120	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	405.00		NIST Webbook
rinpol	417.70		NIST Webbook
rinpol	405.59		NIST Webbook
rinpol	405.00		NIST Webbook
rinpol	2407.00		NIST Webbook
rinpol	2428.00		NIST Webbook
rinpol	405.44		NIST Webbook
rinpol	404.85		NIST Webbook
rinpol	404.64		NIST Webbook
rinpol	403.60		NIST Webbook
rinpol	407.00		NIST Webbook
rinpol	404.40		NIST Webbook
rinpol	404.39		NIST Webbook
rinpol	404.90		NIST Webbook
rinpol	404.72		NIST Webbook
rinpol	409.00		NIST Webbook
tb	746.33	K	Joback Method
tc	1015.64	K	Joback Method
tf	446.25 ± 0.20	K	NIST Webbook
tf	446.13 ± 0.30	K	NIST Webbook
tf	446.78	K	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
vc	0.674	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.63	J/mol×K	1015.64	Joback Method
cpg	474.99	J/mol×K	791.21	Joback Method
cpg	499.53	J/mol×K	880.98	Joback Method
cpg	510.68	J/mol×K	925.87	Joback Method
cpg	521.33	J/mol×K	970.75	Joback Method
cpg	487.69	J/mol×K	836.10	Joback Method
cpg	461.25	J/mol×K	746.33	Joback Method
hsubt	121.60 ± 0.60	kJ/mol	399.00	NIST Webbook
hsubt	125.50 ± 2.10	kJ/mol	383.00	NIST Webbook
hsubt	119.70 ± 5.40	kJ/mol	370.50	NIST Webbook
hsubt	115.50	kJ/mol	398.00	NIST Webbook
hsubt	122.60 ± 0.60	kJ/mol	400.00	NIST Webbook
hvapt	91.40	kJ/mol	585.50	NIST Webbook
psub	6.79e-04	kPa	406.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.71e-04	kPa	402.19	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.53e-04	kPa	402.19	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.53e-04	kPa	402.19	The design, construction, and testing of a new Knudsen effusion apparatus
psub	5.70e-04	kPa	404.34	The design, construction, and testing of a new Knudsen effusion apparatus
psub	5.64e-04	kPa	404.34	The design, construction, and testing of a new Knudsen effusion apparatus
psub	5.65e-04	kPa	404.34	The design, construction, and testing of a new Knudsen effusion apparatus
psub	6.86e-04	kPa	406.35	The design, construction, and testing of a new Knudsen effusion apparatus

psub	3.81e-04	kPa	400.41	The design, construction, and testing of a new Knudsen effusion apparatus
psub	6.80e-04	kPa	406.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	8.10e-04	kPa	408.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	7.96e-04	kPa	408.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	8.00e-04	kPa	408.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	9.62e-04	kPa	410.23	The design, construction, and testing of a new Knudsen effusion apparatus
psub	9.54e-04	kPa	410.23	The design, construction, and testing of a new Knudsen effusion apparatus
psub	9.26e-04	kPa	410.23	The design, construction, and testing of a new Knudsen effusion apparatus
psub	3.94e-04	kPa	400.41	The design, construction, and testing of a new Knudsen effusion apparatus
psub	3.25e-04	kPa	398.22	The design, construction, and testing of a new Knudsen effusion apparatus
psub	3.23e-04	kPa	398.22	The design, construction, and testing of a new Knudsen effusion apparatus
psub	3.25e-04	kPa	398.22	The design, construction, and testing of a new Knudsen effusion apparatus

psub	2.60e-04	kPa	396.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	2.62e-04	kPa	396.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	2.63e-04	kPa	396.35	The design, construction, and testing of a new Knudsen effusion apparatus
psub	2.21e-04	kPa	394.57	The design, construction, and testing of a new Knudsen effusion apparatus
psub	2.34e-04	kPa	394.57	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.77e-04	kPa	392.23	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.79e-04	kPa	392.23	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.49e-04	kPa	390.31	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.52e-04	kPa	390.31	The design, construction, and testing of a new Knudsen effusion apparatus

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The design, construction, and testing of a new Knudsen effusion apparatus:	https://www.doi.org/10.1016/j.jct.2005.08.013

New Knudsen effusion apparatus with simultaneous gravimetric and quartz crystal microbalance measurements of vapour pressure of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method:

<https://www.doi.org/10.1016/j.jct.2010.12.022>

<https://www.doi.org/10.1016/j.jct.2013.11.038>

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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