1-(Methylamino)anthraquinone

Other names:	1-(N-Methylamino)anthraquinone 9,10-Anthracenedione, 1-(methylamino)- «alpha»-Methylaminoanthraquinone Anthraquinone, 1-(methylamino)- C.I. Disperse Red 9 C.I. Solvent Red 111 C.I. 60505 Calco Oil Red ZMQ Celanthrene Red Y Celliton Pink R Diacelliton Fast Pink R Disperse Red 9 Duranol Red GN Macro-lex Red G Methane quinone N-Methyl-1-anthraquinonylamine Oil Red ZMQ Serilene Fast Pink BT Supracet Pink R Waxoline Red MAA Waxoline Red MP 1-(Methylamino)-9,10-anthraquinone 1-(N-Methylamino)-9,10-anthraquinone Anthraquinone, 1-methylamine Amaplast Red AAP Kayaset Red G Macrolex Red GS NSC 3721 Oracet Red G Orient Oil Red 330 Smoke Red M Solvent Red 111
Inchi:	InChI=1S/C15H11NO2/c1-16-12-8-4-7-11-13(12)15(18)10-6-3-2-5-9(10)14(11)17/h2-8,16
InchiKey:	SVTDYSXXLJYUTM-UHFFFAOYSA-N
Formula:	C15H11NO2
SMILES:	CNc1cccc2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	237.25
CAS:	82-38-2

Physical Properties

Property code	Value	Unit	Source
gf	196.12	kJ/mol	Joback Method
hf	-36.91	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.504		Crippen Method
mcvol	176.950	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	803.85	K	Joback Method
tc	1067.96	K	Joback Method
tf	564.01	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.10	J/mol×K	891.89	Joback Method
cpg	566.03	J/mol×K	1067.96	Joback Method
cpg	558.18	J/mol×K	1023.94	Joback Method
cpg	549.27	J/mol×K	979.92	Joback Method
cpg	539.26	J/mol×K	935.91	Joback Method
cpg	502.16	J/mol×K	803.85	Joback Method
cpg	515.75	J/mol×K	847.87	Joback Method
hfust	28.81	kJ/mol	443.20	NIST Webbook
hsubt	123.80 ± 3.30	kJ/mol	394.50	NIST Webbook
hsubt	115.90 ± 3.50	kJ/mol	373.00	NIST Webbook
hsubt	115.00 ± 3.00	kJ/mol	406.00	NIST Webbook
hsubt	115.50 ± 0.40	kJ/mol	461.00	NIST Webbook
hvapt	103.50	kJ/mol	463.00	NIST Webbook

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=C82382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume