9,10-Anthracenedione, 1-amino-

Other names:	1-Amino-9,10-anthraquinone
	1-Aminoanthrachinon
	1-amino-9,10-anthracenedione
	1-aminoanthraquinone
	9,10-Dioxo-9,10-dihydro-1-anthraceneamine
	C.I. 37275
	Diazo Fast Red AL
	NSC 30415
	NSC 458
	Smoke Orange G
	anthraquinone, 1-amino-
	«alpha»-Aminoanthraquinone
	«alpha»-Anthraquinonylamine
Inchi:	InChI=1S/C14H9NO2/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7H,15H2
InchiKey:	KHUFHLFHOQVFGB-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	Nc1cccc2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	223.23
CAS:	82-45-1

Physical Properties

Property code	Value	Unit	Source
gf	164.76	kJ/mol	Joback Method
hf	-35.95	kJ/mol	Joback Method
hfus	22.31	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.044		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	384.41		NIST Webbook
rinpol	386.00		NIST Webbook
rinpol	380.00		NIST Webbook
rinpol	383.68		NIST Webbook
tb	803.33	K	Joback Method
tc	1081.85	K	Joback Method
tf	583.34	K	Joback Method

vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.96	J/mol×K	1081.85	Joback Method
cpg	468.05	J/mol×K	849.75	Joback Method
cpg	479.54	J/mol×K	896.17	Joback Method
cpg	489.82	J/mol×K	942.59	Joback Method
cpg	498.96	J/mol×K	989.01	Joback Method
cpg	506.99	J/mol×K	1035.43	Joback Method
cpg	455.33	J/mol×K	803.33	Joback Method
hfust	28.78	kJ/mol	524.20	NIST Webbook
hfust	28.78	kJ/mol	524.20	NIST Webbook
hsubt	103.30	kJ/mol	513.00	NIST Webbook
hsubt	113.00 ± 0.40	kJ/mol	463.00	NIST Webbook
hsubt	126.50	kJ/mol	428.00	NIST Webbook
hsubt	116.30 ± 3.90	kJ/mol	380.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 1-aminoanthraquinone and 1-nitroanthraquinone in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2016.09.032
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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