1,5-Diaminoanthraquinone

Other names:	9,10-Anthracenedione, 1,5-diamino-
	Anthraquinone, 1,5-diamino-
	C.I. Disperse Red II
	1,5-Anthraquinonyldiamine
	1,5-Daa
	1,5-Diamino-9,10-anthraquinone
	1,5-Diaminoanthrachinon
	NSC 63791
	NSC 7213
	Smoke Red F
Inchi:	InChI=1S/C14H10N2O2/c15-9-5-1-3-7-11(9)14(18)8-4-2-6-10(16)12(8)13(7)17/h1-6H,15
InchiKey:	VWBVCOPVKXNMMZ-UHFFFAOYSA-N
Formula:	C14H10N2O2
SMILES:	Nc1cccc2c1C(=O)c1cccc(N)c1C2=O
Mol. weight [g/mol]:	238.24
CAS:	129-44-2

Physical Properties

Property code	Value	Unit	Source
gf	221.58	kJ/mol	Joback Method
hf	-13.63	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	83.78	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.626		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	880.84	K	Joback Method
tc	1161.76	K	Joback Method
tf	679.12	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.89	J/mol×K	1114.94	Joback Method
cpg	507.63	J/mol×K	880.84	Joback Method
cpg	518.91	J/mol×K	927.66	Joback Method
cpg	528.94	J/mol×K	974.48	Joback Method
cpg	537.75	J/mol×K	1021.30	Joback Method
cpg	545.39	J/mol×K	1068.12	Joback Method
cpg	557.29	J/mol×K	1161.76	Joback Method
hsubt	118.50 ± 4.80	kJ/mol	416.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C129442&Units=SI

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume