

9,10-Anthracenedione, 1,4-diamino-2,3-dihydro-

Other names:

Leuco-1,4-diaminoanthraquinone

Anthraquinone, 1,4-diamino-2,3-dihydro-

1,4-Diamino-2,3-dihydroanthraquinone

Anthraquinone, 2,3-dihydro-1,4-diamino-

Inchi: InChI=1S/C14H12N2O2/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-4H,5

InchiKey: SSGALQHXXKMAJTL-UHFFFAOYSA-N

Formula: C14H12N2O2

SMILES: NC1=C2C(=O)c3ccccc3C(=O)C2=C(N)CC1

Mol. weight [g/mol]: 240.26

CAS: 81-63-0

Physical Properties

Property code	Value	Unit	Source
gf	191.62	kJ/mol	Joback Method
hf	-71.41	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	83.49	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	1.285		Crippen Method
mcvol	177.140	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	881.68	K	Joback Method
tc	1160.22	K	Joback Method
tf	678.36	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.67	J/molxK	881.68	Joback Method
cpg	548.89	J/molxK	928.10	Joback Method
cpg	559.77	J/molxK	974.53	Joback Method
cpg	569.36	J/molxK	1020.95	Joback Method
cpg	577.67	J/molxK	1067.37	Joback Method

cpg	584.76	J/mol×K	1113.80	Joback Method
cpg	590.64	J/mol×K	1160.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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