1,4-Diamino-2,3-dihydroanthraquinone

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:	SSGALQHXKMAJTL-UHFFFAOYSA-N
Formula:	C14H12N2O2
SMILES:	NC1=C2C(=O)c3ccccc3C(=O)C2=C(N)CC1
Mol. weight [g/mol]:	240.26

Physical Properties

Property code	Value	Unit	Source
hf	-26.86	kJ/mol	Cheméo Relay (1.0)
hfus	25.90	kJ/mol	Joback Method
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-3.64		Cheméo Relay (1.0)
logp	1.285		Crippen Method
mcvol	177.140	ml/mol	McGowan Method
tb	654.87	K	Cheméo Relay (1.0)
tf	530.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81630&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point