Anthrarufin, 4,8-dinitro

Other names: 1,5-dihydroxy-4,8-dinitroanthraquinone
Inchi: InChI=1S/C14H6N2O8/c17-7-3-1-5(15(21)22)9-11(7)14(20)10-6(16(23)24)2-4-8(18)12(1
InchiKey: CUIHODIOWPLCMG-UHFFFAOYSA-N
Formula: C14H6N2O8
SMILES: O=C1c2c(O)ccc([N+](=O)[O-])c2C(=O)c2c(O)ccc([N+](=O)[O-])c21
Mol. weight [g/mol]: 330.21
CAS: 128-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-149.46	kJ/mol	Joback Method
hf	-457.35	kJ/mol	Joback Method
hfus	51.01	kJ/mol	Joback Method
hvap	121.71	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	1.690		Crippen Method
mcvol	199.460	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	1200.70	K	Joback Method
tc	1507.79	K	Joback Method
tf	1023.26	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.51	J/mol×K	1200.70	Joback Method
cpg	669.31	J/mol×K	1251.88	Joback Method
cpg	686.45	J/mol×K	1303.06	Joback Method
cpg	705.21	J/mol×K	1354.25	Joback Method
cpg	725.87	J/mol×K	1405.43	Joback Method
cpg	748.70	J/mol×K	1456.61	Joback Method
cpg	773.98	J/mol×K	1507.79	Joback Method

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=C128916&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
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

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