9,10-Anthracenedione, 1,2,5,8-tetrahydroxy-

Other names:	Anthraquinone, 1,2,5,8-tetrahydroxy-
	Alizarinbordeaux
	Alizarine Bordeaux
	Alizarine Bordeaux B
	C.I. Mordant Violet 26
	C.I. 58500
	Khinalizarin
	Quinalizarin
	Quinalizarine
	1,2,5,8-Tetrahydroxy-9,10-anthraquinone
	1,2,5,8-Tetrahydroxyanthraquinone
	Alizarin Bordeaux BD
	1,2,5,8-Tetrahydroxyanthracinon
	1,4,5,6-Tetrahydroxyanthraquinone
	NSC 144046
Inchi:	InChI=1S/C14H8O6/c15-6-3-4-7(16)11-10(6)12(18)5-1-2-8(17)13(19)9(5)14(11)20/h1-4,1
InchiKey:	VBHKTXLEJZIDJF-UHFFFAOYSA-N
Formula:	C14H8O6
SMILES:	O=C1c2ccc(O)c(O)c2C(=O)c2c(O)ccc(O)c21
Mol. weight [g/mol]:	272.21
CAS:	81-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-510.54	kJ/mol	Joback Method
hf	-767.51	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	113.23	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.284		Crippen Method
mcvol	176.360	ml/mol	McGowan Method
pc	7887.21	kPa	Joback Method
tb	1048.30	K	Joback Method
tc	1337.97	K	Joback Method
tf	934.44	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.79	J/mol×K	1048.30	Joback Method
cpg	593.84	J/mol×K	1096.58	Joback Method
cpg	615.29	J/mol×K	1144.86	Joback Method
cpg	639.57	J/mol×K	1193.14	Joback Method
cpg	667.09	J/mol×K	1241.41	Joback Method
cpg	698.26	J/mol×K	1289.69	Joback Method
cpg	733.52	J/mol×K	1337.97	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=C81618&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