

9,10-Anthracenedione, 1,2,4-trihydroxy-

Other names:	Anthraquinone, 1,2,4-trihydroxy- C.I. 58205 C.I. 75410 Hydroxylizaric acid Purpurin Purpurine Smoke Brown G Verantin 1,2,4-Trihydroxyanthraquinone 1,2,4-Trihydroxy-9,10-anthraquinone 1,2,4-Trihydroxyanthrachinon C.I. 1037 1,2,4-Trihydroxy-9,10-anthracenedione 4-Hydroxylizarin
Inchi:	InChI=1S/C14H8O5/c15-8-5-9(16)14(19)11-10(8)12(17)6-3-1-2-4-7(6)13(11)18/h1-5,15-18
InchiKey:	BBNQQADTFFCFGB-UHFFFAOYSA-N
Formula:	C14H8O5
SMILES:	O=C1c2ccccc2C(=O)c2c(O)c(O)cc(O)c21
Mol. weight [g/mol]:	256.21
CAS:	81-54-9

Physical Properties

Property code	Value	Unit	Source
chs	-5866.40	kJ/mol	NIST Webbook
gf	-355.92	kJ/mol	Joback Method
hf	-590.20	kJ/mol	Joback Method
hfus	34.85	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.579		Crippen Method
mcvol	170.490	ml/mol	McGowan Method
pc	6151.48	kPa	Joback Method
tb	967.68	K	Joback Method
tc	1254.11	K	Joback Method
tf	822.72	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.95	J/mol×K	967.68	Joback Method
cpg	539.88	J/mol×K	1015.42	Joback Method
cpg	554.79	J/mol×K	1063.16	Joback Method
cpg	571.00	J/mol×K	1110.89	Joback Method
cpg	588.83	J/mol×K	1158.63	Joback Method
cpg	608.60	J/mol×K	1206.37	Joback Method
cpg	630.61	J/mol×K	1254.11	Joback Method

Sources

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=C81549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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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