1,8-dihydroxy-3-(hydroxymethyl)anthracene-9,10-

Other names: 1,8-dihydroxy-3-hydroxymethylanthraquinone
Inchi: InChI=1S/C15H10O5/c16-6-7-4-9-13(11(18)5-7)15(20)12-8(14(9)19)2-1-3-10(12)17/h1-5
InchiKey: YDQWDHRMZQUTBA-UHFFFAOYSA-N
Formula: C15H10O5
SMILES: O=C1c2cccc(O)c2C(=O)c2c(O)cc(CO)cc21
Mol. weight [g/mol]: 270.24

Physical Properties

Property code	Value	Unit	Source
hfus	35.36	kJ/mol	Joback Method
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	1.365		Crippen Method
mcvol	184.580	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.07	J/mol×K	1007.10	Joback Method
cpg	594.11	J/mol×K	1050.07	Joback Method
cpg	606.42	J/mol×K	1093.04	Joback Method
cpg	619.18	J/mol×K	1136.00	Joback Method
cpg	632.56	J/mol×K	1178.97	Joback Method
cpg	646.71	J/mol×K	1221.94	Joback Method
cpg	661.81	J/mol×K	1264.91	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
Experimental measurement and correlation of the solubility of aloe-emodin in seven pure solvents:	https://www.doi.org/10.1016/j.jct.2016.02.020
Solubility of Aloe-Emodin in Five Imidazolium-Based Ionic Liquids:	https://www.doi.org/10.1021/je400028k

Legend

cpg:	Ideal gas heat capacity
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