2,6-DIHYDROXYANTHRAQUINONE

Other names: 2,6-Dihydroxyanthraquinone
9,10-Anthracenedione, 2,6-dihydroxy-
Anthraflavin
Anthraquinone, 2,6-dihydroxy-
NSC-33531
Inchi: InChI=1S/C14H8O4/c15-7-1-3-9-11(5-7)14(18)10-4-2-8(16)6-12(10)13(9)17/h1-6,15-16H
InchiKey: APAJFZPFBHMFQR-UHFFFAOYSA-N
Formula: C14H8O4
SMILES: O=C1c2ccc(O)cc2C(=O)c2ccc(O)cc21
Mol. weight [g/mol]: 240.21

Physical Properties

Property code	Value	Unit	Source
hf	-433.42	kJ/mol	Cheméo Relay (1.0)
hfus	29.07	kJ/mol	Joback Method
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	1.873		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
tb	676.83	K	Cheméo Relay (1.0)
tf	548.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.36	J/mol×K	887.06	Joback Method
cpg	496.32	J/mol×K	934.29	Joback Method
cpg	508.20	J/mol×K	981.51	Joback Method
cpg	520.20	J/mol×K	1028.74	Joback Method
cpg	532.57	J/mol×K	1075.96	Joback Method
cpg	545.52	J/mol×K	1123.19	Joback Method
cpg	559.27	J/mol×K	1170.41	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84606&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

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