Anthraflavic acid

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
CAS:	84-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-201.30	kJ/mol	Joback Method
hf	-412.89	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.873		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
tb	887.06	K	Joback Method
tc	1170.41	K	Joback Method
tf	711.00	K	Joback Method
vc	0.515	m3/kmol	Joback Method

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:	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=C84606&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