Dihydrooroxylin A

Inchi: InChI=1S/C16H14O5/c1-20-16-11(18)8-13-14(15(16)19)10(17)7-12(21-13)9-5-3-2-4-6-9/
InchiKey: QUAPPCXFYKSDSV-UHFFFAOYSA-N
Formula: C16H14O5
SMILES: COc1c(O)cc2c(c1O)C(=O)CC(c1ccccc1)O2
Mol. weight [g/mol]: 286.28
CAS: 18956-18-8

Physical Properties

Property code	Value	Unit	Source
gf	-284.90	kJ/mol	Joback Method
hf	-613.35	kJ/mol	Joback Method
hfus	40.78	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.813		Crippen Method
mcvol	202.970	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	2762.30		NIST Webbook
rinpol	2762.30		NIST Webbook
tb	918.24	K	Joback Method
tc	1187.19	K	Joback Method
tf	702.84	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.24	J/mol×K	918.24	Joback Method
cpg	654.09	J/mol×K	963.06	Joback Method
cpg	667.49	J/mol×K	1007.89	Joback Method
cpg	680.63	J/mol×K	1052.71	Joback Method
cpg	693.68	J/mol×K	1097.54	Joback Method
cpg	706.84	J/mol×K	1142.36	Joback Method
cpg	720.28	J/mol×K	1187.19	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=C18956188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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