9-Hydroxyselina-4,11-dien-14-oic acid

Inchi: InChI=1S/C15H22O3/c1-9(2)10-7-12-11(14(17)18)5-4-6-15(12,3)13(16)8-10/h10,13,16H
InchiKey: HGHWFNSENQPIOA-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: C=C(C)C1CC2=C(C(=O)O)CCCC2(C)C(O)C1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-177.25	kJ/mol	Joback Method
hf	-503.63	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.905		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1948.00		NIST Webbook
tb	812.64	K	Joback Method
tc	1018.61	K	Joback Method
tf	481.92	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.10	J/mol×K	812.64	Joback Method
cpg	670.15	J/mol×K	846.97	Joback Method
cpg	684.79	J/mol×K	881.30	Joback Method
cpg	699.15	J/mol×K	915.63	Joback Method
cpg	713.33	J/mol×K	949.96	Joback Method
cpg	727.48	J/mol×K	984.29	Joback Method
cpg	741.70	J/mol×K	1018.61	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=R390577&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