«beta»-Selinen-2«alpha»-ol (Jatamol A)

Inchi: InChI=1S/C15H24O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)14(16)9-12/h12-14,16H,1,3,5-9
InchiKey: BFMDGLARCCRBDW-LRMYVUMKSA-N
Formula: C15H24O
SMILES: C=C(C)C1CC(O)C2(C)CCCC(=C)C2C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	123.16	kJ/mol	Joback Method
hf	-209.76	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	63.98	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1690.00		NIST Webbook
tb	651.96	K	Joback Method
tc	859.17	K	Joback Method
tf	354.81	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/mol×K	651.96	Joback Method
cpg	592.62	J/mol×K	686.50	Joback Method
cpg	611.16	J/mol×K	721.03	Joback Method
cpg	628.80	J/mol×K	755.57	Joback Method
cpg	645.67	J/mol×K	790.10	Joback Method
cpg	661.88	J/mol×K	824.64	Joback Method
cpg	677.55	J/mol×K	859.17	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=R232901&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume