Laciniata ether A

Inchi: InChI=1S/C15H22O2/c1-6-14(4)9-8-13(17-14)15(5)10-7-12(16-15)11(2)3/h6,8,12H,1-2,7
InchiKey: SNZFUKFLMNBJGL-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=CC1(C)CC=C(C2(C)CCC(C(=C)C)O2)O1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	145.05	kJ/mol	Joback Method
hf	-198.45	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.749		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	620.25	K	Joback Method
tc	853.60	K	Joback Method
tf	373.11	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.85	J/mol×K	620.25	Joback Method
cpg	566.48	J/mol×K	659.14	Joback Method
cpg	585.93	J/mol×K	698.03	Joback Method
cpg	604.49	J/mol×K	736.93	Joback Method
cpg	622.43	J/mol×K	775.82	Joback Method
cpg	640.06	J/mol×K	814.71	Joback Method
cpg	657.65	J/mol×K	853.60	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=R226738&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