Davana ether (Isomer)

Inchi: InChI=1S/C15H24O2/c1-6-15(5)10-8-13(17-15)11(2)12-7-9-14(3,4)16-12/h6,13H,1,7-10H
InchiKey: JEMPCTQTARBZOI-VAWYXSNFSA-N
Formula: C15H24O2
SMILES: C=CC1(C)CCC(C(C)=C2CCC(C)(C)O2)O1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	82.34	kJ/mol	Joback Method
hf	-294.16	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.973		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	626.07	K	Joback Method
tc	858.37	K	Joback Method
tf	371.95	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.45	J/mol×K	626.07	Joback Method
cpg	589.98	J/mol×K	664.79	Joback Method
cpg	610.33	J/mol×K	703.50	Joback Method
cpg	629.78	J/mol×K	742.22	Joback Method
cpg	648.62	J/mol×K	780.94	Joback Method
cpg	667.13	J/mol×K	819.66	Joback Method
cpg	685.61	J/mol×K	858.37	Joback Method

Sources

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=R342206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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