Davana ether, isomer # 3

Inchi: InChI=1S/C15H22O2/c1-6-15(5)10-8-13(17-15)11(2)12-7-9-14(3,4)16-12/h6-7,9,13H,1,8
InchiKey: ZFMNPTVNDZBEHA-VAWYXSNFSA-N
Formula: C15H22O2
SMILES: C=CC1(C)CCC(C(C)=C2C=CC(C)(C)O2)O1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	112.30	kJ/mol	Joback Method
hf	-236.38	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.749		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1535.00		NIST Webbook
tb	625.23	K	Joback Method
tc	859.75	K	Joback Method
tf	372.71	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.73	J/mol×K	625.23	Joback Method
cpg	567.15	J/mol×K	664.32	Joback Method
cpg	586.42	J/mol×K	703.40	Joback Method
cpg	604.84	J/mol×K	742.49	Joback Method
cpg	622.71	J/mol×K	781.57	Joback Method
cpg	640.32	J/mol×K	820.66	Joback Method
cpg	657.97	J/mol×K	859.75	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=R593429&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