

Davana ether

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:	<chem>C=CC1(C)CCC(C(C)=C2C=CC(C)(C)O2)O1</chem>
Mol. weight [g/mol]:	234.33
CAS:	35470-57-6

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	1474.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1497.50		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1497.50		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1514.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35470576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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