Phellandrenol

Inchi: InChI=1S/C10H16O/c1-8-3-5-10(6-4-8)9(2)7-11/h3-5,9-11H,6-7H2,1-2H3
InchiKey: DBERZDFDAKEFPP-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CCC(C(C)CO)C=C1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-31.20	kJ/mol	Joback Method
hf	-248.83	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.137		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1235.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1814.00		NIST Webbook
tb	542.79	K	Joback Method
tc	737.22	K	Joback Method
tf	269.70	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.08	J/mol×K	542.79	Joback Method
cpg	396.43	J/mol×K	704.82	Joback Method
cpg	384.95	J/mol×K	672.41	Joback Method
cpg	372.79	J/mol×K	640.01	Joback Method
cpg	359.95	J/mol×K	607.60	Joback Method
cpg	346.39	J/mol×K	575.20	Joback Method
cpg	407.26	J/mol×K	737.22	Joback Method

dvisc	0.0001118	Pa×s	542.79	Joback Method
dvisc	0.0001821	Pa×s	497.27	Joback Method
dvisc	0.0003271	Pa×s	451.76	Joback Method
dvisc	0.0006699	Pa×s	406.25	Joback Method
dvisc	0.0016443	Pa×s	360.73	Joback Method
dvisc	0.0052306	Pa×s	315.21	Joback Method
dvisc	0.0245888	Pa×s	269.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R291524&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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