Farnesol (E), methyl ether

Inchi: InChI=1S/C16H28O/c1-14(2)8-6-9-15(3)10-7-11-16(4)12-13-17-5/h8,10,12H,6-7,9,11,13
InchiKey: HZDZRGKULMGCJE-NCZFFCEISA-N
Formula: C16H28O
SMILES: COCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	193.85	kJ/mol	Joback Method
hf	-183.50	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.052		Crippen Method
mcvol	229.270	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	1683.90		NIST Webbook
tb	600.02	K	Joback Method
tc	784.01	K	Joback Method
tf	235.19	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.43	J/mol×K	600.02	Joback Method
cpg	604.02	J/mol×K	630.68	Joback Method
cpg	621.71	J/mol×K	661.35	Joback Method
cpg	638.54	J/mol×K	692.01	Joback Method
cpg	654.57	J/mol×K	722.68	Joback Method
cpg	669.84	J/mol×K	753.34	Joback Method
cpg	684.39	J/mol×K	784.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352673&Units=SI

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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