Farnesol formate

Inchi: InChI=1S/C16H26O2/c1-14(2)7-5-8-15(3)9-6-10-16(4)11-12-18-13-17/h7,9,11,13H,5-6,8
InchiKey: KSBAOYWMHJTPQU-XGGJEREUSA-N
Formula: C16H26O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCOC=O
Mol. weight [g/mol]: 250.38
CAS: 917105-98-7

Physical Properties

Property code	Value	Unit	Source
gf	94.33	kJ/mol	Joback Method
hf	-269.08	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.579		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1736.50		NIST Webbook
rinpol	1736.50		NIST Webbook
tb	648.68	K	Joback Method
tc	836.41	K	Joback Method
tf	277.19	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.72	J/mol×K	648.68	Joback Method
cpg	628.65	J/mol×K	679.97	Joback Method
cpg	644.72	J/mol×K	711.26	Joback Method
cpg	659.99	J/mol×K	742.54	Joback Method
cpg	674.51	J/mol×K	773.83	Joback Method
cpg	688.31	J/mol×K	805.12	Joback Method
cpg	701.47	J/mol×K	836.41	Joback Method

Sources

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=C917105987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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