3,7,11-Trimethyldodecylacetate

Other names: Hexahydrofarnesyl acetate
Inchi: InChI=1S/C17H34O2/c1-14(2)8-6-9-15(3)10-7-11-16(4)12-13-19-17(5)18/h14-16H,6-13H
InchiKey: FMIKGNLHOCVXJO-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CC(=O)OCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	-148.98	kJ/mol	Joback Method
hf	-654.85	kJ/mol	Joback Method
hfus	32.00	kJ/mol	Joback Method
hvap	61.43	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	5.208		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2122.00		NIST Webbook
tb	663.33	K	Joback Method
tc	837.31	K	Joback Method
tf	308.51	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.46	J/mol×K	663.33	Joback Method
cpg	752.60	J/mol×K	692.33	Joback Method
cpg	770.87	J/mol×K	721.32	Joback Method
cpg	788.28	J/mol×K	750.32	Joback Method
cpg	804.86	J/mol×K	779.31	Joback Method

cpg	820.61	J/mol×K	808.31	Joback Method
cpg	835.57	J/mol×K	837.31	Joback Method
dvisc	0.0054749	Pa×s	308.51	Joback Method
dvisc	0.0015723	Pa×s	367.65	Joback Method
dvisc	0.0006381	Pa×s	426.78	Joback Method
dvisc	0.0003225	Pa×s	485.92	Joback Method
dvisc	0.0001890	Pa×s	545.06	Joback Method
dvisc	0.0001230	Pa×s	604.19	Joback Method
dvisc	0.0000864	Pa×s	663.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374104&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

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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