Hexanoic acid, 3,5,5-trimethyl-, cyclohexylmethyl ester

Inchi: InChI=1S/C16H30O2/c1-13(11-16(2,3)4)10-15(17)18-12-14-8-6-5-7-9-14/h13-14H,5-12H

InchiKey: ZYKBYSOILBDXIW-UHFFFAOYSA-N

Formula: C16H30O2

SMILES: CC(CC(=O)OCC1CCCCC1)CC(C)(C)C

Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
gf	-125.23	kJ/mol	Joback Method
hf	-578.08	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.572		Crippen Method
mcvol	232.880	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	657.65	K	Joback Method
tc	860.54	K	Joback Method
tf	337.04	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.63	J/mol×K	657.65	Joback Method
cpg	695.34	J/mol×K	691.47	Joback Method
cpg	715.75	J/mol×K	725.28	Joback Method
cpg	734.92	J/mol×K	759.10	Joback Method
cpg	752.89	J/mol×K	792.91	Joback Method
cpg	769.70	J/mol×K	826.73	Joback Method
cpg	785.40	J/mol×K	860.54	Joback Method
dvisc	0.0043452	Pa×s	337.04	Joback Method

dvisc	0.0015194	Pa×s	390.48	Joback Method
dvisc	0.0006842	Pa×s	443.91	Joback Method
dvisc	0.0003657	Pa×s	497.35	Joback Method
dvisc	0.0002208	Pa×s	550.78	Joback Method
dvisc	0.0001457	Pa×s	604.21	Joback Method
dvisc	0.0001029	Pa×s	657.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406823&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume