

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

Inchi:	InChI=1S/C16H32O2/c1-6-7-8-9-10-11-18-15(17)12-14(2)13-16(3,4)5/h14H,6-13H2,1-5H
InchiKey:	CRMRELGFIDICVHJ-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	256.42

Physical Properties

Property code	Value	Unit	Source
gf	-149.68	kJ/mol	Joback Method
hf	-632.40	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.962		Crippen Method
mvol	243.740	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	638.10	K	Joback Method
tc	814.57	K	Joback Method
tf	329.66	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.66	J/molxK	638.10	Joback Method
cpg	763.92	J/molxK	785.16	Joback Method
cpg	748.54	J/molxK	755.75	Joback Method
cpg	732.36	J/molxK	726.34	Joback Method
cpg	715.34	J/molxK	696.92	Joback Method
cpg	697.45	J/molxK	667.51	Joback Method
cpg	778.51	J/molxK	814.57	Joback Method
dvisc	0.0000987	Paxs	638.10	Joback Method

dvisc	0.0001385	Paxs	586.69	Joback Method
dvisc	0.0002072	Paxs	535.29	Joback Method
dvisc	0.0003379	Paxs	483.88	Joback Method
dvisc	0.0006189	Paxs	432.47	Joback Method
dvisc	0.0013347	Paxs	381.07	Joback Method
dvisc	0.0036579	Paxs	329.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406058&Units=SI

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

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