

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

Inchi:	InChI=1S/C19H38O2/c1-6-7-8-9-10-11-12-13-14-21-18(20)15-17(2)16-19(3,4)5/h17H,6-
InchiKey:	GIFONBUKXIYAFO-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	298.50

Physical Properties

Property code	Value	Unit	Source
gf	-124.42	kJ/mol	Joback Method
hf	-694.32	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	6.133		Crippen Method
mvol	286.010	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	706.74	K	Joback Method
tc	882.45	K	Joback Method
tf	363.47	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.89	J/molxK	706.74	Joback Method
cpg	940.32	J/molxK	853.17	Joback Method
cpg	924.23	J/molxK	823.88	Joback Method
cpg	907.28	J/molxK	794.60	Joback Method
cpg	889.43	J/molxK	765.31	Joback Method
cpg	870.65	J/molxK	736.03	Joback Method
cpg	955.57	J/molxK	882.45	Joback Method
dvisc	0.0000648	Paxs	706.74	Joback Method

dvisc	0.0000913	Paxs	649.53	Joback Method
dvisc	0.0001374	Paxs	592.32	Joback Method
dvisc	0.0002255	Paxs	535.11	Joback Method
dvisc	0.0004168	Paxs	477.89	Joback Method
dvisc	0.0009106	Paxs	420.68	Joback Method
dvisc	0.0025443	Paxs	363.47	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=U406061&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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