

Hexanoic acid, 3,5,5-trimethyl-, dec-2-yl ester

Inchi:	InChI=1S/C19H38O2/c1-7-8-9-10-11-12-13-17(3)21-18(20)14-16(2)15-19(4,5)6/h16-17H
InchiKey:	PBWYOKHVLIHEJN-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCC(C)OC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	298.50

Physical Properties

Property code	Value	Unit	Source
gf	-126.86	kJ/mol	Joback Method
hf	-699.60	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.131		Crippen Method
mvol	286.010	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook
tb	706.30	K	Joback Method
tc	884.00	K	Joback Method
tf	348.47	K	Joback Method
vc	1.101	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.31	J/molxK	706.30	Joback Method
cpg	871.32	J/molxK	735.92	Joback Method
cpg	890.32	J/molxK	765.53	Joback Method
cpg	908.36	J/molxK	795.15	Joback Method
cpg	925.47	J/molxK	824.77	Joback Method
cpg	941.70	J/molxK	854.38	Joback Method
cpg	957.06	J/molxK	884.00	Joback Method
dvisc	0.0034336	Paxs	348.47	Joback Method

dvisc	0.0010684	Paxs	408.11	Joback Method
dvisc	0.0004477	Paxs	467.75	Joback Method
dvisc	0.0002284	Paxs	527.38	Joback Method
dvisc	0.0001336	Paxs	587.02	Joback Method
dvisc	0.0000863	Paxs	646.66	Joback Method
dvisc	0.0000600	Paxs	706.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406826&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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