

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

Inchi:	InChI=1S/C15H30O2/c1-6-7-8-9-10-17-14(16)11-13(2)12-15(3,4)5/h13H,6-12H2,1-5H3
InchiKey:	QMINKKOXQXKWDS-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	242.40

Physical Properties

Property code	Value	Unit	Source
gf	-158.10	kJ/mol	Joback Method
hf	-611.76	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	56.46	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.572		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
tb	615.22	K	Joback Method
tc	792.72	K	Joback Method
tf	318.39	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.69	J/molxK	615.22	Joback Method
cpg	707.28	J/molxK	763.14	Joback Method
cpg	692.20	J/molxK	733.56	Joback Method
cpg	676.33	J/molxK	703.97	Joback Method
cpg	659.64	J/molxK	674.39	Joback Method
cpg	642.10	J/molxK	644.80	Joback Method
cpg	721.60	J/molxK	792.72	Joback Method
dvisc	0.0001128	Paxs	615.22	Joback Method
dvisc	0.0001580	Paxs	565.75	Joback Method
dvisc	0.0002360	Paxs	516.28	Joback Method

dvisc	0.0003838	Paxs	466.81	Joback Method
dvisc	0.0007005	Paxs	417.33	Joback Method
dvisc	0.0015032	Paxs	367.86	Joback Method
dvisc	0.0040895	Paxs	318.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406057&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

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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