

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

Inchi:	InChI=1S/C12H24O2/c1-6-7-14-11(13)8-10(2)9-12(3,4)5/h10H,6-9H2,1-5H3
InchiKey:	TXDNNEFZLUFLRT-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	200.32

Physical Properties

Property code	Value	Unit	Source
gf	-183.36	kJ/mol	Joback Method
hf	-549.84	kJ/mol	Joback Method
hfus	18.69	kJ/mol	Joback Method
hvap	49.78	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.402		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
tb	546.58	K	Joback Method
tc	728.79	K	Joback Method
tf	284.58	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.33	J/molxK	546.58	Joback Method
cpg	544.39	J/molxK	698.42	Joback Method
cpg	530.48	J/molxK	668.05	Joback Method
cpg	515.84	J/molxK	637.68	Joback Method
cpg	500.46	J/molxK	607.32	Joback Method
cpg	484.29	J/molxK	576.95	Joback Method
cpg	557.59	J/molxK	728.79	Joback Method
dvisc	0.0001638	Paxs	546.58	Joback Method
dvisc	0.0002282	Paxs	502.91	Joback Method
dvisc	0.0003386	Paxs	459.25	Joback Method

dvisc	0.0005458	Paxs	415.58	Joback Method
dvisc	0.0009843	Paxs	371.91	Joback Method
dvisc	0.0020765	Paxs	328.25	Joback Method
dvisc	0.0055085	Paxs	284.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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