

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

Inchi:	InChI=1S/C16H32O2/c1-7-8-9-10-14(3)18-15(17)11-13(2)12-16(4,5)6/h13-14H,7-12H2,1
InchiKey:	JCMIYHNMLWJKNR-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCC(C)OC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	256.42

Physical Properties

Property code	Value	Unit	Source
gf	-152.12	kJ/mol	Joback Method
hf	-637.68	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.961		Crippen Method
mvol	243.740	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	637.66	K	Joback Method
tc	816.85	K	Joback Method
tf	314.66	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.03	J/molxK	637.66	Joback Method
cpg	765.60	J/molxK	786.99	Joback Method
cpg	750.03	J/molxK	757.12	Joback Method
cpg	733.62	J/molxK	727.26	Joback Method
cpg	716.33	J/molxK	697.39	Joback Method
cpg	698.15	J/molxK	667.53	Joback Method
cpg	780.35	J/molxK	816.85	Joback Method
dvisc	0.0000919	Paxs	637.66	Joback Method

dvisc	0.0001319	Paxs	583.83	Joback Method
dvisc	0.0002038	Paxs	529.99	Joback Method
dvisc	0.0003475	Paxs	476.16	Joback Method
dvisc	0.0006789	Paxs	422.33	Joback Method
dvisc	0.0016128	Paxs	368.49	Joback Method
dvisc	0.0051517	Paxs	314.66	Joback Method

Sources

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=U406821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
h_{vap}:	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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