

Tricaproin

Other names:

Hexanoic acid, 1,2,3-propanetriyl ester
Hexanoin, tri-
Caproic triglyceride
Glycerol tricaproate
Glyceryl tricaproate
Tricapronin
Trihexanoin
Trihexanoyl glycerol
Glycerol trihexanoate
Hexanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester
NSC 406885
Tricaproylglycerol

Inchi: InChI=1S/C21H38O6/c1-4-7-10-13-19(22)25-16-18(27-21(24)15-12-9-6-3)17-26-20(23)1**InchiKey:** MAYCICSNZYXLHB-UHFFFAOYSA-N**Formula:** C21H38O6**SMILES:** CCCCCC(=O)OCC(COC(=O)CCCC)OC(=O)CCCC**Mol. weight [g/mol]:** 386.52**CAS:** 621-70-5

Physical Properties

Property code	Value	Unit	Source
gf	-578.26	kJ/mol	Joback Method
hf	-1216.45	kJ/mol	Joback Method
hfus	54.98	kJ/mol	Joback Method
hvap	108.30 ± 3.80	kJ/mol	NIST Webbook
log10ws	-5.31		Crippen Method
logp	4.725		Crippen Method
mcvol	329.070	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
tb	908.31	K	Joback Method
tc	1112.06	K	Joback Method
tf	527.91	K	Joback Method
vc	1.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.93	J/molxK	1112.06	Joback Method
cpg	1153.94	J/molxK	1078.10	Joback Method
cpg	1142.60	J/molxK	1044.15	Joback Method
cpg	1129.91	J/molxK	1010.19	Joback Method
cpg	1115.85	J/molxK	976.23	Joback Method
cpg	1100.42	J/molxK	942.27	Joback Method
cpg	1083.61	J/molxK	908.31	Joback Method
cpl	753.00	J/molxK	313.00	NIST Webbook
dvisc	0.0000295	Paxs	908.31	Joback Method
dvisc	0.0004481	Paxs	527.91	Joback Method
dvisc	0.0000391	Paxs	844.91	Joback Method
dvisc	0.0000544	Paxs	781.51	Joback Method
dvisc	0.0000801	Paxs	718.11	Joback Method
dvisc	0.0001273	Paxs	654.71	Joback Method
dvisc	0.0002232	Paxs	591.31	Joback Method
hvapt	94.20	kJ/mol	383.00	NIST Webbook
hvapt	99.90	kJ/mol	349.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621705&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
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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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