

1,2,3-Propanetriol, tripropanoate

Other names:	Tripropionin
	Propionin, tri-
	Glycerine tripropionate
	Glycerol tripropionate
	Glyceryl tripropionate
	Tripropionine
	1,2,3-Propanetriol, tripropionate
	1,2,3-Propanetriol, 1,2,3-tripropanoate
	NSC 36744
	Tripropionylglycerol
Inchi:	InChI=1S/C12H20O6/c1-4-10(13)16-7-9(18-12(15)6-3)8-17-11(14)5-2/h9H,4-8H2,1-3H3
InchiKey:	YZWRNSARCRTXDS-UHFFFAOYSA-N
Formula:	C12H20O6
SMILES:	CCC(=O)OCC(COC(=O)CC)OC(=O)CC
Mol. weight [g/mol]:	260.28
CAS:	139-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-654.04	kJ/mol	Joback Method
hf	-1030.69	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	91.40 ± 0.40	kJ/mol	NIST Webbook
hvap	91.36 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.55		Crippen Method
logp	1.215		Crippen Method
mcvol	202.260	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	702.39	K	Joback Method
tc	889.54	K	Joback Method
tf	426.48	K	Joback Method

vc	0.773	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.41	J/mol×K	702.39	Joback Method
cpg	633.36	J/mol×K	889.54	Joback Method
cpg	623.61	J/mol×K	858.34	Joback Method
cpg	613.08	J/mol×K	827.15	Joback Method
cpg	601.78	J/mol×K	795.96	Joback Method
cpg	589.73	J/mol×K	764.77	Joback Method
cpg	576.94	J/mol×K	733.58	Joback Method
cpl	481.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0001077	Pa×s	702.39	Joback Method
dvisc	0.0001394	Pa×s	656.40	Joback Method
dvisc	0.0001875	Pa×s	610.42	Joback Method
dvisc	0.0002647	Pa×s	564.43	Joback Method
dvisc	0.0003972	Pa×s	518.45	Joback Method
dvisc	0.0006451	Pa×s	472.47	Joback Method
dvisc	0.0011632	Pa×s	426.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C139457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
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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