

Diglycolic acid, propyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C15H28O5/c1-6-7-19-13(16)10-18-11-14(17)20-9-12(2)8-15(3,4)5/h12H,6-11H
InchiKey:	BSRINQJLJHQQSK-UHFFFAOYSA-N
Formula:	C15H28O5
SMILES:	CCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	288.38

Physical Properties

Property code	Value	Unit	Source
gf	-497.02	kJ/mol	Joback Method
hf	-988.78	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.572		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpola	2190.00		NIST Webbook
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tb	713.93	K	Joback Method
tc	898.50	K	Joback Method
tf	412.78	K	Joback Method
vc	0.924	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.41	J/molxK	713.93	Joback Method
cpg	725.84	J/molxK	744.69	Joback Method
cpg	741.38	J/molxK	775.45	Joback Method
cpg	756.04	J/molxK	806.22	Joback Method
cpg	769.83	J/molxK	836.98	Joback Method
cpg	782.75	J/molxK	867.74	Joback Method
cpg	794.83	J/molxK	898.50	Joback Method
dvisc	0.0011564	Paxs	412.78	Joback Method

dvisc	0.0005456	Paxs	462.97	Joback Method
dvisc	0.0002982	Paxs	513.16	Joback Method
dvisc	0.0001815	Paxs	563.36	Joback Method
dvisc	0.0001198	Paxs	613.55	Joback Method
dvisc	0.0000842	Paxs	663.74	Joback Method
dvisc	0.0000622	Paxs	713.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382036&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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