

Glycerol, 2,3-dimethyl, 1-(14-methylpentadecanoate)

Inchi:	InChI=1S/C21H42O4/c1-19(2)15-13-11-9-7-5-6-8-10-12-14-16-21(22)25-18-20(24-4)17-2
InchiKey:	RRFJHCAFBDDEFJJ-UHFFFAOYSA-N
Formula:	C21H42O4
SMILES:	COCC(COC(=O)CCCCCCCCCCCCC(C)C)OC
Mol. weight [g/mol]:	358.56

Physical Properties

Property code	Value	Unit	Source
gf	-322.86	kJ/mol	Joback Method
hf	-996.57	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	75.54	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.528		Crippen Method
mvol	325.930	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	800.13	K	Joback Method
tc	981.54	K	Joback Method
tf	413.05	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.84	J/molxK	800.13	Joback Method
cpg	1125.56	J/molxK	951.30	Joback Method
cpg	1110.01	J/molxK	921.07	Joback Method
cpg	1093.38	J/molxK	890.83	Joback Method
cpg	1075.65	J/molxK	860.60	Joback Method
cpg	1056.80	J/molxK	830.36	Joback Method
cpg	1140.02	J/molxK	981.54	Joback Method
dvisc	0.0000305	Paxs	800.13	Joback Method

dvisc	0.0000423	Paxs	735.62	Joback Method
dvisc	0.0000624	Paxs	671.10	Joback Method
dvisc	0.0001000	Paxs	606.59	Joback Method
dvisc	0.0001794	Paxs	542.08	Joback Method
dvisc	0.0003765	Paxs	477.56	Joback Method
dvisc	0.0009966	Paxs	413.05	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=R56446&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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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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