

Diglycolic acid, di(3-methylpent-2-yl) ester

Inchi:	InChI=1S/C16H30O5/c1-7-11(3)13(5)20-15(17)9-19-10-16(18)21-14(6)12(4)8-2/h11-14H
InchiKey:	IASDDMMXUYNFNO-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CCC(C)C(C)OC(=O)COCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-498.76	kJ/mol	Joback Method
hf	-1016.51	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.959		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpola	2282.00		NIST Webbook
rinpola	2282.00		NIST Webbook
tb	738.72	K	Joback Method
tc	923.60	K	Joback Method
tf	376.63	K	Joback Method
vc	0.974	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.61	J/molxK	738.72	Joback Method
cpg	841.65	J/molxK	892.79	Joback Method
cpg	828.35	J/molxK	861.97	Joback Method
cpg	814.09	J/molxK	831.16	Joback Method
cpg	798.88	J/molxK	800.35	Joback Method
cpg	782.72	J/molxK	769.53	Joback Method
cpg	853.99	J/molxK	923.60	Joback Method
dvisc	0.0000510	Paxs	738.72	Joback Method

dvisc	0.0000717	Paxs	678.37	Joback Method
dvisc	0.0001077	Paxs	618.02	Joback Method
dvisc	0.0001767	Paxs	557.67	Joback Method
dvisc	0.0003269	Paxs	497.33	Joback Method
dvisc	0.0007166	Paxs	436.98	Joback Method
dvisc	0.0020206	Paxs	376.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381881&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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