

Diglycolic acid, isobutyl isoheptyl ester

Inchi:	InChI=1S/C14H26O5/c1-11(2)6-5-7-18-13(15)9-17-10-14(16)19-8-12(3)4/h11-12H,5-10H
InchiKey:	YOKKQZQEJUFTJM-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	274.35

Physical Properties

Property code	Value	Unit	Source
gf	-510.72	kJ/mol	Joback Method
hf	-964.67	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.182		Crippen Method
mvol	228.870	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2159.00		NIST Webbook
rinpol	2159.00		NIST Webbook
tb	693.84	K	Joback Method
tc	874.69	K	Joback Method
tf	384.09	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.96	J/molxK	693.84	Joback Method
cpg	667.87	J/molxK	723.98	Joback Method
cpg	682.99	J/molxK	754.12	Joback Method
cpg	697.31	J/molxK	784.26	Joback Method
cpg	710.83	J/molxK	814.40	Joback Method
cpg	723.55	J/molxK	844.55	Joback Method
cpg	735.46	J/molxK	874.69	Joback Method
dvisc	0.0015512	Paxs	384.09	Joback Method

dvisc	0.0007036	Paxs	435.72	Joback Method
dvisc	0.0003773	Paxs	487.34	Joback Method
dvisc	0.0002280	Paxs	538.97	Joback Method
dvisc	0.0001504	Paxs	590.59	Joback Method
dvisc	0.0001061	Paxs	642.22	Joback Method
dvisc	0.0000789	Paxs	693.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

Latest version available from:

<https://www.chemeo.com/cid/82-596-0/Diglycolic-acid-isobutyl-isohehexyl-ester.pdf>

Generated by Cheméo on 2024-04-27 23:49:25.188377614 +0000 UTC m=+16551014.108954929.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.