

Diglycolic acid, isobutyl pentyl ester

Inchi:	InChI=1S/C13H24O5/c1-4-5-6-7-17-12(14)9-16-10-13(15)18-8-11(2)3/h11H,4-10H2,1-3H
InchiKey:	LSVDSRUHUBTIQ-UHFFFAOYSA-N
Formula:	C13H24O5
SMILES:	CCCCCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	260.33

Physical Properties

Property code	Value	Unit	Source
gf	-516.70	kJ/mol	Joback Method
hf	-938.75	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.936		Crippen Method
mvol	214.780	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
tb	671.40	K	Joback Method
tc	850.36	K	Joback Method
tf	387.82	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.96	J/molxK	671.40	Joback Method
cpg	612.15	J/molxK	701.23	Joback Method
cpg	626.63	J/molxK	731.05	Joback Method
cpg	640.40	J/molxK	760.88	Joback Method
cpg	653.44	J/molxK	790.71	Joback Method
cpg	665.75	J/molxK	820.53	Joback Method
cpg	677.33	J/molxK	850.36	Joback Method
dvisc	0.0013703	Paxs	387.82	Joback Method

dvisc	0.0006936	Paxs	435.08	Joback Method
dvisc	0.0004012	Paxs	482.35	Joback Method
dvisc	0.0002559	Paxs	529.61	Joback Method
dvisc	0.0001757	Paxs	576.87	Joback Method
dvisc	0.0001277	Paxs	624.14	Joback Method
dvisc	0.0000971	Paxs	671.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382127&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

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
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

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