

Diglycolic acid, isobutyl 2-pentyl ester

Inchi:	InChI=1S/C13H24O5/c1-5-6-11(4)18-13(15)9-16-8-12(14)17-7-10(2)3/h10-11H,5-9H2,1-
InchiKey:	DTDIQGBHSLYSEM-UHFFFAOYSA-N
Formula:	C13H24O5
SMILES:	CCCC(C)OC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	260.33

Physical Properties

Property code	Value	Unit	Source
gf	-519.14	kJ/mol	Joback Method
hf	-944.03	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.934		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	670.96	K	Joback Method
tc	852.46	K	Joback Method
tf	372.82	K	Joback Method
vc	0.818	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.43	J/molxK	670.96	Joback Method
cpg	612.87	J/molxK	701.21	Joback Method
cpg	627.57	J/molxK	731.46	Joback Method
cpg	641.52	J/molxK	761.71	Joback Method
cpg	654.72	J/molxK	791.96	Joback Method
cpg	667.17	J/molxK	822.21	Joback Method
cpg	678.85	J/molxK	852.46	Joback Method
dvisc	0.0017069	Paxs	372.82	Joback Method

dvisc	0.0007834	Paxs	422.51	Joback Method
dvisc	0.0004236	Paxs	472.20	Joback Method
dvisc	0.0002575	Paxs	521.89	Joback Method
dvisc	0.0001707	Paxs	571.58	Joback Method
dvisc	0.0001208	Paxs	621.27	Joback Method
dvisc	0.0000900	Paxs	670.96	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=U382333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	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

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