

Diglycolic acid, isobutyl 3-phenylpropyl ester

Inchi:	InChI=1S/C17H24O5/c1-14(2)11-22-17(19)13-20-12-16(18)21-10-6-9-15-7-4-3-5-8-15/h3
InchiKey:	OAZLVVHNOHXPBE-UHFFFAOYSA-N
Formula:	C17H24O5
SMILES:	CC(C)COC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	308.37

Physical Properties

Property code	Value	Unit	Source
gf	-370.61	kJ/mol	Joback Method
hf	-784.78	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.378		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpola	2798.00		NIST Webbook
rinpola	2798.00		NIST Webbook
tb	789.60	K	Joback Method
tc	991.44	K	Joback Method
tf	459.32	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.03	J/molxK	789.60	Joback Method
cpg	749.32	J/molxK	823.24	Joback Method
cpg	763.52	J/molxK	856.88	Joback Method
cpg	776.64	J/molxK	890.52	Joback Method
cpg	788.68	J/molxK	924.16	Joback Method
cpg	799.66	J/molxK	957.80	Joback Method
cpg	809.57	J/molxK	991.44	Joback Method
dvisc	0.0007568	Paxs	459.32	Joback Method

dvisc	0.0003904	Paxs	514.37	Joback Method
dvisc	0.0002289	Paxs	569.41	Joback Method
dvisc	0.0001474	Paxs	624.46	Joback Method
dvisc	0.0001020	Paxs	679.51	Joback Method
dvisc	0.0000746	Paxs	734.55	Joback Method
dvisc	0.0000569	Paxs	789.60	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=U382171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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