

Diglycolic acid, isohexyl 3-methylphenyl ester

Inchi:	InChI=1S/C17H24O5/c1-13(2)6-5-9-21-16(18)11-20-12-17(19)22-15-8-4-7-14(3)10-15/h
InchiKey:	TXNJLQXDUPNJPN-UHFFFAOYSA-N
Formula:	C17H24O5
SMILES:	<chem>Cc1cccc(OC(=O)COCC(=O)OCCCC(C)C)c1</chem>
Mol. weight [g/mol]:	308.37

Physical Properties

Property code	Value	Unit	Source
gf	-380.24	kJ/mol	Joback Method
hf	-796.25	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.896		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	794.58	K	Joback Method
tc	997.23	K	Joback Method
tf	471.84	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.23	J/molxK	794.58	Joback Method
cpg	748.43	J/molxK	828.36	Joback Method
cpg	762.53	J/molxK	862.13	Joback Method
cpg	775.55	J/molxK	895.91	Joback Method
cpg	787.49	J/molxK	929.68	Joback Method
cpg	798.35	J/molxK	963.46	Joback Method
cpg	808.13	J/molxK	997.23	Joback Method
dvisc	0.0006330	Paxs	471.84	Joback Method

dvisc	0.0003456	Paxs	525.63	Joback Method
dvisc	0.0002112	Paxs	579.42	Joback Method
dvisc	0.0001403	Paxs	633.21	Joback Method
dvisc	0.0000994	Paxs	687.00	Joback Method
dvisc	0.0000740	Paxs	740.79	Joback Method
dvisc	0.0000573	Paxs	794.58	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=U382102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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