

Diglycolic acid, isohexyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H28O5/c1-16(2)8-6-12-23-18(20)14-22-15-19(21)24-13-7-11-17-9-4-3-5-10
InchiKey:	YMPSKPASOXLNMY-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-353.77	kJ/mol	Joback Method
hf	-826.06	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.158		Crippen Method
mvol	275.560	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	3096.00		NIST Webbook
tb	835.36	K	Joback Method
tc	1036.71	K	Joback Method
tf	481.86	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.41	J/molxK	835.36	Joback Method
cpg	916.10	J/molxK	1003.15	Joback Method
cpg	905.07	J/molxK	969.59	Joback Method
cpg	892.90	J/molxK	936.03	Joback Method
cpg	879.57	J/molxK	902.48	Joback Method
cpg	865.08	J/molxK	868.92	Joback Method
cpg	925.99	J/molxK	1036.71	Joback Method
dvisc	0.0000429	Paxs	835.36	Joback Method
dvisc	0.0000565	Paxs	776.44	Joback Method

dvisc	0.0000779	Paxs	717.53	Joback Method
dvisc	0.0001136	Paxs	658.61	Joback Method
dvisc	0.0001785	Paxs	599.69	Joback Method
dvisc	0.0003094	Paxs	540.78	Joback Method
dvisc	0.0006138	Paxs	481.86	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=U382174&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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