

Diglycolic acid, isohexyl phenethyl ester

Inchi:	InChI=1S/C18H26O5/c1-15(2)7-6-11-22-17(19)13-21-14-18(20)23-12-10-16-8-4-3-5-9-16
InchiKey:	LEHYWCKTYWWALT-UHFFFAOYSA-N
Formula:	C18H26O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	322.40

Physical Properties

Property code	Value	Unit	Source
gf	-362.19	kJ/mol	Joback Method
hf	-805.42	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.768		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	2961.00		NIST Webbook
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tb	812.48	K	Joback Method
tc	1013.76	K	Joback Method
tf	470.59	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.30	J/molxK	812.48	Joback Method
cpg	857.53	J/molxK	980.21	Joback Method
cpg	846.51	J/molxK	946.66	Joback Method
cpg	834.39	J/molxK	913.12	Joback Method
cpg	821.15	J/molxK	879.57	Joback Method
cpg	806.79	J/molxK	846.03	Joback Method
cpg	867.46	J/molxK	1013.76	Joback Method
dvisc	0.0000495	Paxs	812.48	Joback Method

dvisc	0.0000650	Paxs	755.50	Joback Method
dvisc	0.0000892	Paxs	698.52	Joback Method
dvisc	0.0001296	Paxs	641.53	Joback Method
dvisc	0.0002025	Paxs	584.55	Joback Method
dvisc	0.0003483	Paxs	527.57	Joback Method
dvisc	0.0006831	Paxs	470.59	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=U382160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
m_cvol:	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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