Diglycolic acid, isohexyl 4-methoxybenzyl ester

Inchi: InChI=1S/C18H26O6/c1-14(2)5-4-10-23-17(19)12-22-13-18(20)24-11-15-6-8-16(21-3)9-7

InchiKey: UNBLDHMKGLEBEI-UHFFFAOYSA-N

Formula: C18H26O6

SMILES: COc1ccc(COC(=O)COCC(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-476.82	kJ/mol	Joback Method
hf	-949.11	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	81.34	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.734		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	3145.00		NIST Webbook
rinpol	3145.00		NIST Webbook
tb	839.88	K	Joback Method
tc	1042.54	K	Joback Method
tf	505.34	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.17	J/mol×K	839.88	Joback Method
cpg	881.45	J/mol×K	1008.76	Joback Method
cpg	871.45	J/mol×K	974.98	Joback Method
cpg	860.21	J/mol×K	941.21	Joback Method
cpg	847.75	J/mol×K	907.43	Joback Method
cpg	834.06	J/mol×K	873.66	Joback Method
cpg	890.21	J/mol×K	1042.54	Joback Method
dvisc	0.0000375	Pa×s	839.88	Joback Method

dvisc	0.0000484	Pa×s	784.12	Joback Method
dvisc	0.0000649	Pa×s	728.37	Joback Method
dvisc	0.0000914	Pa×s	672.61	Joback Method
dvisc	0.0001369	Pa×s	616.85	Joback Method
dvisc	0.0002221	Pa×s	561.10	Joback Method
dvisc	0.0004011	Pa×s	505.34	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=U382250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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