Diglycolic acid, 2,6-dimethoxyphenyl isohexyl ester

Inchi: InChI=1S/C18H26O7/c1-13(2)7-6-10-24-16(19)11-23-12-17(20)25-18-14(21-3)8-5-9-15(1

InchiKey: AKMIURKZNIMYIK-UHFFFAOYSA-N

Formula: C18H26O7

SMILES: COc1cccc(OC)c1OC(=O)COCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 354.39

Physical Properties

Property code	Value	Unit	Source
gf	-591.45	kJ/mol	Joback Method
hf	-1092.80	kJ/mol	Joback Method
hfus	41.25	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.605		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	3062.00		NIST Webbook
rinpol	3062.00		NIST Webbook
tb	867.28	K	Joback Method
tc	1071.89	K	Joback Method
tf	540.09	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.67	J/mol×K	867.28	Joback Method
cpg	860.89	J/mol×K	901.38	Joback Method
cpg	873.78	J/mol×K	935.48	Joback Method
cpg	885.31	J/mol×K	969.58	Joback Method
cpg	895.46	J/mol×K	1003.68	Joback Method
cpg	904.21	J/mol×K	1037.79	Joback Method
cpg	911.51	J/mol×K	1071.89	Joback Method
dvisc	0.0002439	Pa×s	540.09	Joback Method

dvisc	0.0001447	Pa×s	594.62	Joback Method
dvisc	0.0000937	Pa×s	649.15	Joback Method
dvisc	0.0000649	Pa×s	703.68	Joback Method
dvisc	0.0000474	Pa×s	758.22	Joback Method
dvisc	0.0000361	Pa×s	812.75	Joback Method
dvisc	0.0000284	Pa×s	867.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U381907&Units=SI

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