Diglycolic acid, 2,5-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C18H26O5/c1-13(2)6-5-9-22-17(19)11-21-12-18(20)23-16-10-14(3)7-8-15(16)4

InchiKey: NKGTXEPZAXTTLA-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: Cc1ccc(C)c(OC(=O)COCC(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-381.45	kJ/mol	Joback Method
hf	-828.36	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	79.60	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.205		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	822.44	K	Joback Method
tc	1025.37	K	Joback Method
tf	495.63	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.76	J/mol×K	822.44	Joback Method
cpg	805.07	J/mol×K	856.26	Joback Method
cpg	819.24	J/mol×K	890.08	Joback Method
cpg	832.27	J/mol×K	923.90	Joback Method
cpg	844.17	J/mol×K	957.73	Joback Method
cpg	854.92	J/mol×K	991.55	Joback Method
cpg	864.54	J/mol×K	1025.37	Joback Method
dvisc	0.0004891	Pa×s	495.63	Joback Method

dvisc	0.0002778	Pa×s	550.10	Joback Method
dvisc	0.0001747	Pa×s	604.57	Joback Method
dvisc	0.0001186	Pa×s	659.03	Joback Method
dvisc	0.0000854	Pa×s	713.50	Joback Method
dvisc	0.0000644	Pa×s	767.97	Joback Method
dvisc	0.0000505	Pa×s	822.44	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=U382707&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