Diglycolic acid, hexyl 2-methylphenyl ester

Inchi: InChI=1S/C17H24O5/c1-3-4-5-8-11-21-16(18)12-20-13-17(19)22-15-10-7-6-9-14(15)2/h6
InchiKey: KORLGFROKQGEON-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCCCCCOC(=O)COCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-377.80	kJ/mol	Joback Method
hf	-790.97	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.041		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	795.02	K	Joback Method
tc	995.27	K	Joback Method
tf	486.84	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.69	J/mol×K	795.02	Joback Method
cpg	747.70	J/mol×K	828.40	Joback Method
cpg	761.66	J/mol×K	861.77	Joback Method
cpg	774.58	J/mol×K	895.15	Joback Method
cpg	786.44	J/mol×K	928.52	Joback Method
cpg	797.27	J/mol×K	961.90	Joback Method
cpg	807.05	J/mol×K	995.27	Joback Method
dvisc	0.0005581	Pa×s	486.84	Joback Method

dvisc	0.0003254	Pa×s	538.20	Joback Method
dvisc	0.0002084	Pa×s	589.57	Joback Method
dvisc	0.0001434	Pa×s	640.93	Joback Method
dvisc	0.0001043	Pa×s	692.29	Joback Method
dvisc	0.0000792	Pa×s	743.66	Joback Method
dvisc	0.0000624	Pa×s	795.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382009&Units=SI
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

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