Diglycolic acid, 4-bromophenyl isohexyl ester

Inchi: InChI=1S/C16H21BrO5/c1-12(2)4-3-9-21-15(18)10-20-11-16(19)22-14-7-5-13(17)6-8-14/
InchiKey: XUXZNCOYLBAUDC-UHFFFAOYSA-N
Formula: C16H21BrO5
SMILES: CC(C)CCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 373.24

Physical Properties

Property code	Value	Unit	Source
gf	-374.34	kJ/mol	Joback Method
hf	-749.28	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	80.92	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.350		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2976.00		NIST Webbook
rinpol	2976.00		NIST Webbook
tb	837.86	K	Joback Method
tc	1051.85	K	Joback Method
tf	520.37	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.12	J/mol×K	837.86	Joback Method
cpg	728.34	J/mol×K	873.53	Joback Method
cpg	740.45	J/mol×K	909.19	Joback Method
cpg	751.47	J/mol×K	944.86	Joback Method
cpg	761.40	J/mol×K	980.52	Joback Method
cpg	770.25	J/mol×K	1016.19	Joback Method
cpg	778.03	J/mol×K	1051.85	Joback Method
dvisc	0.0004628	Pa×s	520.37	Joback Method

dvisc	0.0002728	Pa×s	573.28	Joback Method
dvisc	0.0001758	Pa×s	626.20	Joback Method
dvisc	0.0001213	Pa×s	679.12	Joback Method
dvisc	0.0000883	Pa×s	732.03	Joback Method
dvisc	0.0000671	Pa×s	784.94	Joback Method
dvisc	0.0000528	Pa×s	837.86	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=U381897&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