Diglycolic acid, 4-bromophenyl octyl ester

Inchi: InChI=1S/C18H25BrO5/c1-2-3-4-5-6-7-12-23-17(20)13-22-14-18(21)24-16-10-8-15(19)9-
InchiKey: ASBBAPAXLKSLJE-UHFFFAOYSA-N
Formula: C18H25BrO5
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 401.29

Physical Properties

Property code	Value	Unit	Source
gf	-355.06	kJ/mol	Joback Method
hf	-785.28	kJ/mol	Joback Method
hfus	48.07	kJ/mol	Joback Method
hvap	85.76	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.275		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	884.06	K	Joback Method
tc	1095.00	K	Joback Method
tf	557.91	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.89	J/mol×K	884.06	Joback Method
cpg	884.90	J/mol×K	1059.85	Joback Method
cpg	875.96	J/mol×K	1024.69	Joback Method
cpg	865.90	J/mol×K	989.53	Joback Method
cpg	854.71	J/mol×K	954.37	Joback Method
cpg	842.38	J/mol×K	919.22	Joback Method
cpg	892.74	J/mol×K	1095.00	Joback Method
dvisc	0.0000429	Pa×s	884.06	Joback Method

dvisc	0.0000541	Pa×s	829.70	Joback Method
dvisc	0.0000705	Pa×s	775.34	Joback Method
dvisc	0.0000957	Pa×s	720.98	Joback Method
dvisc	0.0001363	Pa×s	666.63	Joback Method
dvisc	0.0002068	Pa×s	612.27	Joback Method
dvisc	0.0003404	Pa×s	557.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381900&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