Diglycolic acid, 4-chlorobenzyl octyl ester

Inchi: InChI=1S/C19H27ClO5/c1-2-3-4-5-6-7-12-24-18(21)14-23-15-19(22)25-13-16-8-10-17(20
InchiKey: MCRZBZXQCMTAFE-UHFFFAOYSA-N
Formula: C19H27ClO5
SMILES: CCCCCCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 370.87

Physical Properties

Property code	Value	Unit	Source
gf	-372.89	kJ/mol	Joback Method
hf	-847.99	kJ/mol	Joback Method
hfus	49.58	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.303		Crippen Method
mcvol	287.800	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3364.00		NIST Webbook
tb	878.21	K	Joback Method
tc	1083.90	K	Joback Method
tf	539.30	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.61	J/mol×K	878.21	Joback Method
cpg	888.85	J/mol×K	912.49	Joback Method
cpg	901.90	J/mol×K	946.77	Joback Method
cpg	913.75	J/mol×K	981.06	Joback Method
cpg	924.43	J/mol×K	1015.34	Joback Method
cpg	933.95	J/mol×K	1049.62	Joback Method
cpg	942.31	J/mol×K	1083.90	Joback Method
dvisc	0.0003777	Pa×s	539.30	Joback Method

dvisc	0.0002186	Pa×s	595.78	Joback Method
dvisc	0.0001390	Pa×s	652.27	Joback Method
dvisc	0.0000951	Pa×s	708.75	Joback Method
dvisc	0.0000688	Pa×s	765.24	Joback Method
dvisc	0.0000520	Pa×s	821.72	Joback Method
dvisc	0.0000408	Pa×s	878.21	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=U382261&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