Diglycolic acid, 4-chlorobenzyl butyl ester

Inchi: InChI=1S/C15H19ClO5/c1-2-3-8-20-14(17)10-19-11-15(18)21-9-12-4-6-13(16)7-5-12/h4-
InchiKey: CGHQYYYLFOHJOR-UHFFFAOYSA-N
Formula: C15H19ClO5
SMILES: CCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 314.76

Physical Properties

Property code	Value	Unit	Source
gf	-406.57	kJ/mol	Joback Method
hf	-765.43	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.743		Crippen Method
mcvol	231.440	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	786.69	K	Joback Method
tc	992.98	K	Joback Method
tf	494.22	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.85	J/mol×K	786.69	Joback Method
cpg	703.51	J/mol×K	958.60	Joback Method
cpg	694.17	J/mol×K	924.22	Joback Method
cpg	683.83	J/mol×K	889.84	Joback Method
cpg	672.50	J/mol×K	855.45	Joback Method
cpg	660.17	J/mol×K	821.07	Joback Method
cpg	711.86	J/mol×K	992.98	Joback Method
dvisc	0.0000717	Pa×s	786.69	Joback Method

dvisc	0.0000902	Pa×s	737.94	Joback Method
dvisc	0.0001173	Pa×s	689.20	Joback Method
dvisc	0.0001586	Pa×s	640.45	Joback Method
dvisc	0.0002255	Pa×s	591.71	Joback Method
dvisc	0.0003415	Pa×s	542.97	Joback Method
dvisc	0.0005613	Pa×s	494.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382256&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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