Diglycolic acid, 4-chlorobenzyl isohexyl ester

Inchi: InChI=1S/C17H23ClO5/c1-13(2)4-3-9-22-16(19)11-21-12-17(20)23-10-14-5-7-15(18)8-6-

InchiKey: JKTPPCJQHBFJMF-UHFFFAOYSA-N

Formula: C17H23ClO5

SMILES: CC(C)CCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-392.17	kJ/mol	Joback Method
hf	-811.99	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	81.09	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.379		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	832.01	K	Joback Method
tc	1038.87	K	Joback Method
tf	501.76	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.60	J/mol×K	832.01	Joback Method
cpg	773.58	J/mol×K	866.49	Joback Method
cpg	786.43	J/mol×K	900.96	Joback Method
cpg	798.17	J/mol×K	935.44	Joback Method
cpg	808.79	J/mol×K	969.92	Joback Method
cpg	818.31	J/mol×K	1004.39	Joback Method
cpg	826.72	J/mol×K	1038.87	Joback Method
dvisc	0.0005186	Pa×s	501.76	Joback Method

dvisc	0.0002894	Pa×s	556.80	Joback Method
dvisc	0.0001794	Pa×s	611.84	Joback Method
dvisc	0.0001203	Pa×s	666.88	Joback Method
dvisc	0.0000857	Pa×s	721.93	Joback Method
dvisc	0.0000641	Pa×s	776.97	Joback Method
dvisc	0.0000498	Pa×s	832.01	Joback Method

Sources

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=U382258&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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