Diglycolic acid, 4-chlorobenzyl hexyl ester

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

InchiKey: UYQDRSZOPXMLML-UHFFFAOYSA-N

Formula: C17H23ClO5

SMILES: CCCCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-389.73	kJ/mol	Joback Method
hf	-806.71	kJ/mol	Joback Method
hfus	44.40	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.523		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	832.45	K	Joback Method
tc	1037.10	K	Joback Method
tf	516.76	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.04	J/mol×K	832.45	Joback Method
cpg	817.41	J/mol×K	1002.99	Joback Method
cpg	807.90	J/mol×K	968.88	Joback Method
cpg	797.31	J/mol×K	934.78	Joback Method
cpg	785.64	J/mol×K	900.67	Joback Method
cpg	772.88	J/mol×K	866.56	Joback Method
cpg	825.85	J/mol×K	1037.10	Joback Method
dvisc	0.0000543	Pa×s	832.45	Joback Method

dvisc	0.0000689	Pa×s	779.83	Joback Method
dvisc	0.0000903	Pa×s	727.22	Joback Method
dvisc	0.0001236	Pa×s	674.61	Joback Method
dvisc	0.0001783	Pa×s	621.99	Joback Method
dvisc	0.0002753	Pa×s	569.38	Joback Method
dvisc	0.0004644	Pa×s	516.76	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=U382259&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