

Diglycolic acid, 4-chlorobenzyl pentyl ester

Inchi:	InChI=1S/C16H21ClO5/c1-2-3-4-9-21-15(18)11-20-12-16(19)22-10-13-5-7-14(17)8-6-13
InchiKey:	MPBRMDYZINQWGZ-UHFFFAOYSA-N
Formula:	C16H21ClO5
SMILES:	CCCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	328.79

Physical Properties

Property code	Value	Unit	Source
gf	-398.15	kJ/mol	Joback Method
hf	-786.07	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.133		Crippen Method
mvol	245.530	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2987.00		NIST Webbook
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tb	809.57	K	Joback Method
tc	1014.73	K	Joback Method
tf	505.49	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.49	J/molxK	809.57	Joback Method
cpg	716.09	J/molxK	843.76	Joback Method
cpg	728.65	J/molxK	877.96	Joback Method
cpg	740.17	J/molxK	912.15	Joback Method
cpg	750.66	J/molxK	946.34	Joback Method
cpg	760.11	J/molxK	980.54	Joback Method
cpg	768.53	J/molxK	1014.73	Joback Method
dvisc	0.0005117	Paxs	505.49	Joback Method

dvisc	0.0003073	Paxs	556.17	Joback Method
dvisc	0.0002009	Paxs	606.85	Joback Method
dvisc	0.0001403	Paxs	657.53	Joback Method
dvisc	0.0001031	Paxs	708.21	Joback Method
dvisc	0.0000790	Paxs	758.89	Joback Method
dvisc	0.0000625	Paxs	809.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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