

Diglycolic acid, 4-chlorobenzyl decyl ester

Inchi:	InChI=1S/C21H31ClO5/c1-2-3-4-5-6-7-8-9-14-26-20(23)16-25-17-21(24)27-15-18-10-12
InchiKey:	LNWUEUDZTRVYAT-UHFFFAOYSA-N
Formula:	C21H31ClO5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	398.92

Physical Properties

Property code	Value	Unit	Source
gf	-356.05	kJ/mol	Joback Method
hf	-889.27	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	90.38	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.084		Crippen Method
mvol	315.980	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	3604.00		NIST Webbook
rinpol	3604.00		NIST Webbook
tb	923.97	K	Joback Method
tc	1133.80	K	Joback Method
tf	561.84	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.98	J/molxK	923.97	Joback Method
cpg	1052.76	J/molxK	1098.83	Joback Method
cpg	1043.39	J/molxK	1063.86	Joback Method
cpg	1032.75	J/molxK	1028.89	Joback Method
cpg	1020.81	J/molxK	993.91	Joback Method
cpg	1007.56	J/molxK	958.94	Joback Method
cpg	1060.86	J/molxK	1133.80	Joback Method
dvisc	0.0000303	Paxs	923.97	Joback Method

dvisc	0.0000389	Paxs	863.62	Joback Method
dvisc	0.0000518	Paxs	803.26	Joback Method
dvisc	0.0000723	Paxs	742.90	Joback Method
dvisc	0.0001071	Paxs	682.55	Joback Method
dvisc	0.0001712	Paxs	622.20	Joback Method
dvisc	0.0003027	Paxs	561.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382263&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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