

Diglycolic acid, 4-chlorobenzyl nonyl ester

Inchi:	InChI=1S/C20H29ClO5/c1-2-3-4-5-6-7-8-13-25-19(22)15-24-16-20(23)26-14-17-9-11-18
InchiKey:	LCKGRVJKRUMRKM-UHFFFAOYSA-N
Formula:	C20H29ClO5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	384.89

Physical Properties

Property code	Value	Unit	Source
gf	-364.47	kJ/mol	Joback Method
hf	-868.63	kJ/mol	Joback Method
hfus	52.17	kJ/mol	Joback Method
hvap	88.16	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.694		Crippen Method
mvol	301.890	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	3475.00		NIST Webbook
rinpol	3475.00		NIST Webbook
tb	901.09	K	Joback Method
tc	1108.44	K	Joback Method
tf	550.57	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.48	J/molxK	901.09	Joback Method
cpg	993.10	J/molxK	1073.88	Joback Method
cpg	983.64	J/molxK	1039.32	Joback Method
cpg	972.96	J/molxK	1004.76	Joback Method
cpg	961.05	J/molxK	970.21	Joback Method
cpg	947.89	J/molxK	935.65	Joback Method
cpg	1001.35	J/molxK	1108.44	Joback Method
dvisc	0.0000352	Paxs	901.09	Joback Method

dvisc	0.0000450	Paxs	842.67	Joback Method
dvisc	0.0000598	Paxs	784.25	Joback Method
dvisc	0.0000830	Paxs	725.83	Joback Method
dvisc	0.0001222	Paxs	667.41	Joback Method
dvisc	0.0001938	Paxs	608.99	Joback Method
dvisc	0.0003387	Paxs	550.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382262&Units=SI

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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