

Diglycolic acid, 4-chlorophenyl nonyl ester

Inchi:	InChI=1S/C19H27ClO5/c1-2-3-4-5-6-7-8-13-24-18(21)14-23-15-19(22)25-17-11-9-16(20)
InchiKey:	BOSSPZZDFAJSQD-UHFFFAOYSA-N
Formula:	C19H27ClO5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	370.87

Physical Properties

Property code	Value	Unit	Source
gf	-372.89	kJ/mol	Joback Method
hf	-847.99	kJ/mol	Joback Method
hfus	49.58	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.556		Crippen Method
mvol	287.800	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	3254.00		NIST Webbook
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tb	878.21	K	Joback Method
tc	1083.90	K	Joback Method
tf	539.30	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.61	J/molxK	878.21	Joback Method
cpg	933.95	J/molxK	1049.62	Joback Method
cpg	924.43	J/molxK	1015.34	Joback Method
cpg	913.75	J/molxK	981.06	Joback Method
cpg	901.90	J/molxK	946.77	Joback Method
cpg	888.85	J/molxK	912.49	Joback Method
cpg	942.31	J/molxK	1083.90	Joback Method
dvisc	0.0000408	Paxs	878.21	Joback Method

dvisc	0.0000520	Paxs	821.72	Joback Method
dvisc	0.0000688	Paxs	765.24	Joback Method
dvisc	0.0000951	Paxs	708.75	Joback Method
dvisc	0.0001390	Paxs	652.27	Joback Method
dvisc	0.0002186	Paxs	595.78	Joback Method
dvisc	0.0003777	Paxs	539.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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