

Diglycolic acid, 3-chlorophenyl octyl ester

Inchi:	InChI=1S/C18H25ClO5/c1-2-3-4-5-6-7-11-23-17(20)13-22-14-18(21)24-16-10-8-9-15(19)
InchiKey:	RXZRIKCHJRHIII-UHFFFAOYSA-N
Formula:	C18H25ClO5
SMILES:	CCCCCCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	356.84

Physical Properties

Property code	Value	Unit	Source
gf	-381.31	kJ/mol	Joback Method
hf	-827.35	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.166		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	3116.00		NIST Webbook
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tb	855.33	K	Joback Method
tc	1060.14	K	Joback Method
tf	528.03	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.44	J/molxK	855.33	Joback Method
cpg	875.37	J/molxK	1026.01	Joback Method
cpg	865.84	J/molxK	991.87	Joback Method
cpg	855.18	J/molxK	957.74	Joback Method
cpg	843.41	J/molxK	923.60	Joback Method
cpg	830.50	J/molxK	889.47	Joback Method
cpg	883.79	J/molxK	1060.14	Joback Method
dvisc	0.0000471	Paxs	855.33	Joback Method

dvisc	0.0000599	Paxs	800.78	Joback Method
dvisc	0.0000789	Paxs	746.23	Joback Method
dvisc	0.0001086	Paxs	691.68	Joback Method
dvisc	0.0001577	Paxs	637.13	Joback Method
dvisc	0.0002457	Paxs	582.58	Joback Method
dvisc	0.0004196	Paxs	528.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381772&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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