

Diglycolic acid, 4-chloro-2-methylphenyl hexyl ester

Inchi:	InChI=1S/C17H23ClO5/c1-3-4-5-6-9-22-16(19)11-21-12-17(20)23-15-8-7-14(18)10-13(15)
InchiKey:	DRQYRDFZIXIMAH-UHFFFAOYSA-N
Formula:	C17H23ClO5
SMILES:	CCCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	342.81

Physical Properties

Property code	Value	Unit	Source
gf	-399.36	kJ/mol	Joback Method
hf	-818.18	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.694		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2956.00		NIST Webbook
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tb	837.43	K	Joback Method
tc	1042.91	K	Joback Method
tf	529.28	K	Joback Method
vc	0.995	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.01	J/molxK	837.43	Joback Method
cpg	771.77	J/molxK	871.68	Joback Method
cpg	784.43	J/molxK	905.92	Joback Method
cpg	796.00	J/molxK	940.17	Joback Method
cpg	806.47	J/molxK	974.41	Joback Method
cpg	815.84	J/molxK	1008.66	Joback Method
cpg	824.12	J/molxK	1042.91	Joback Method
dvisc	0.0004050	Paxs	529.28	Joback Method

dvisc	0.0002506	Paxs	580.64	Joback Method
dvisc	0.0001677	Paxs	632.00	Joback Method
dvisc	0.0001192	Paxs	683.36	Joback Method
dvisc	0.0000888	Paxs	734.71	Joback Method
dvisc	0.0000688	Paxs	786.07	Joback Method
dvisc	0.0000550	Paxs	837.43	Joback Method

Sources

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=U382743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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