

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

Inchi:	InChI=1S/C15H19ClO5/c1-3-4-7-20-14(17)9-19-10-15(18)21-13-6-5-12(16)8-11(13)2/h5-
InchiKey:	JILYNDNUVLATGE-UHFFFAOYSA-N
Formula:	C15H19ClO5
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	314.76

Physical Properties

Property code	Value	Unit	Source
gf	-416.20	kJ/mol	Joback Method
hf	-776.90	kJ/mol	Joback Method
hfus	38.83	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.914		Crippen Method
mcvol	231.440	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2697.00		NIST Webbook
rinpol	2697.00		NIST Webbook
tb	791.67	K	Joback Method
tc	998.75	K	Joback Method
tf	506.74	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.71	J/molxK	791.67	Joback Method
cpg	658.94	J/molxK	826.18	Joback Method
cpg	671.19	J/molxK	860.70	Joback Method
cpg	682.43	J/molxK	895.21	Joback Method
cpg	692.67	J/molxK	929.73	Joback Method
cpg	701.90	J/molxK	964.24	Joback Method
cpg	710.12	J/molxK	998.75	Joback Method
dvisc	0.0004861	Paxs	506.74	Joback Method

dvisc	0.0003088	Paxs	554.23	Joback Method
dvisc	0.0002107	Paxs	601.72	Joback Method
dvisc	0.0001520	Paxs	649.20	Joback Method
dvisc	0.0001147	Paxs	696.69	Joback Method
dvisc	0.0000897	Paxs	744.18	Joback Method
dvisc	0.0000723	Paxs	791.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382740&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

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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