Diglycolic acid, di(2,6-dichlorophenyl) ester

Inchi: InChI=1S/C16H10Cl4O5/c17-9-3-1-4-10(18)15(9)24-13(21)7-23-8-14(22)25-16-11(19)5-2
InchiKey: ZPQQCOKUFJXGTG-UHFFFAOYSA-N
Formula: C16H10Cl4O5
SMILES: O=C(COCC(=O)Oc1c(Cl)cccc1Cl)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 424.06

Physical Properties

Property code	Value	Unit	Source
gf	-350.42	kJ/mol	Joback Method
hf	-631.17	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	96.67	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.828		Crippen Method
mcvol	258.490	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	3508.00		NIST Webbook
rinpol	3508.00		NIST Webbook
tb	963.48	K	Joback Method
tc	1209.13	K	Joback Method
tf	659.23	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.89	J/mol×K	963.48	Joback Method
cpg	662.88	J/mol×K	1004.42	Joback Method
cpg	668.53	J/mol×K	1045.36	Joback Method
cpg	672.83	J/mol×K	1086.30	Joback Method
cpg	675.78	J/mol×K	1127.24	Joback Method
cpg	677.36	J/mol×K	1168.18	Joback Method
cpg	677.58	J/mol×K	1209.13	Joback Method
dvisc	0.0002003	Pa×s	659.23	Joback Method

dvisc	0.0001413	Pa×s	709.94	Joback Method
dvisc	0.0001044	Pa×s	760.65	Joback Method
dvisc	0.0000801	Pa×s	811.36	Joback Method
dvisc	0.0000634	Pa×s	862.06	Joback Method
dvisc	0.0000515	Pa×s	912.77	Joback Method
dvisc	0.0000428	Pa×s	963.48	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382305&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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