Diglycolic acid, 2,4-dichloro-6-formylphenyl ethyl ester

Inchi: InChI=1S/C13H12Cl2O6/c1-2-20-11(17)6-19-7-12(18)21-13-8(5-16)3-9(14)4-10(13)15/h3

InchiKey: DHYPOBHZANLWMJ-UHFFFAOYSA-N

Formula: C13H12Cl2O6

SMILES: CCOC(=O)COCC(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 335.14

Physical Properties

Property code	Value	Unit	Source
gf	-554.12	kJ/mol	Joback Method
hf	-848.41	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	85.01	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.291		Crippen Method
mcvol	217.070	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	836.98	K	Joback Method
tc	1054.85	K	Joback Method
tf	568.64	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.08	J/mol×K	836.98	Joback Method
cpg	605.93	J/mol×K	1018.54	Joback Method
cpg	600.37	J/mol×K	982.23	Joback Method
cpg	593.79	J/mol×K	945.92	Joback Method
cpg	586.20	J/mol×K	909.60	Joback Method
cpg	577.62	J/mol×K	873.29	Joback Method
cpg	610.44	J/mol×K	1054.85	Joback Method
dvisc	0.0000911	Pa×s	836.98	Joback Method

dvisc	0.0001101	Pa×s	792.26	Joback Method
dvisc	0.0001361	Pa×s	747.53	Joback Method
dvisc	0.0001729	Pa×s	702.81	Joback Method
dvisc	0.0002268	Pa×s	658.09	Joback Method
dvisc	0.0003096	Pa×s	613.36	Joback Method
dvisc	0.0004438	Pa×s	568.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U382629&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

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