Adipic acid, ethyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C14H15Cl3O4/c1-2-20-11(18)5-3-4-6-12(19)21-14-10(16)8-7-9(15)13(14)17/h7
InchiKey: KYTYHBCTSPGHQS-UHFFFAOYSA-N
Formula: C14H15Cl3O4
SMILES: CCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 353.62

Physical Properties

Property code	Value	Unit	Source
gf	-353.11	kJ/mol	Joback Method
hf	-666.99	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.676		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	826.21	K	Joback Method
tc	1043.90	K	Joback Method
tf	545.60	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/mol×K	826.21	Joback Method
cpg	655.24	J/mol×K	1007.62	Joback Method
cpg	648.02	J/mol×K	971.34	Joback Method
cpg	639.87	J/mol×K	935.06	Joback Method
cpg	630.78	J/mol×K	898.77	Joback Method
cpg	620.76	J/mol×K	862.49	Joback Method
cpg	661.54	J/mol×K	1043.90	Joback Method
dvisc	0.0000845	Pa×s	826.21	Joback Method
dvisc	0.0001033	Pa×s	779.44	Joback Method

dvisc	0.0001294	Pa×s	732.67	Joback Method
dvisc	0.0001673	Pa×s	685.90	Joback Method
dvisc	0.0002246	Pa×s	639.14	Joback Method
dvisc	0.0003158	Pa×s	592.37	Joback Method
dvisc	0.0004707	Pa×s	545.60	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=U353931&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