2-Ethylbutyric acid, 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C12H13Cl3O2/c1-3-7(4-2)12(16)17-10-6-8(13)5-9(14)11(10)15/h5-7H,3-4H2,1
InchiKey: QKHFAMMRYMHVQR-UHFFFAOYSA-N
Formula: C12H13Cl3O2
SMILES: CCC(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 295.59

Physical Properties

Property code	Value	Unit	Source
gf	-138.47	kJ/mol	Joback Method
hf	-386.19	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.988		Crippen Method
mcvol	200.340	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	703.72	K	Joback Method
tc	927.03	K	Joback Method
tf	435.90	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.65	J/mol×K	703.72	Joback Method
cpg	481.68	J/mol×K	740.94	Joback Method
cpg	492.90	J/mol×K	778.16	Joback Method
cpg	503.31	J/mol×K	815.38	Joback Method
cpg	512.94	J/mol×K	852.60	Joback Method
cpg	521.80	J/mol×K	889.81	Joback Method
cpg	529.90	J/mol×K	927.03	Joback Method
dvisc	0.0009519	Pa×s	435.90	Joback Method

dvisc	0.0005906	Pa×s	480.54	Joback Method
dvisc	0.0003974	Pa×s	525.17	Joback Method
dvisc	0.0002845	Pa×s	569.81	Joback Method
dvisc	0.0002138	Pa×s	614.45	Joback Method
dvisc	0.0001670	Pa×s	659.08	Joback Method
dvisc	0.0001346	Pa×s	703.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370559&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

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