

2-Ethylbutyric acid, 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C12H13Cl3O2/c1-3-7(4-2)12(16)17-11-9(14)6-5-8(13)10(11)15/h5-7H,3-4H2,1
InchiKey:	SKBYZFGVQZKWAE-UHFFFAOYSA-N
Formula:	C12H13Cl3O2
SMILES:	CCC(CC)C(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	295.59
CAS:	58516-55-5

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	1859.00		NIST Webbook
tb	703.72	K	Joback Method
tc	927.03	K	Joback Method
tf	435.90	K	Joback Method
vc	0.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005906	Paxs	480.54	Joback Method
dvisc	0.0003974	Paxs	525.17	Joback Method
dvisc	0.0002845	Paxs	569.81	Joback Method
dvisc	0.0002138	Paxs	614.45	Joback Method
dvisc	0.0001670	Paxs	659.08	Joback Method
dvisc	0.0001346	Paxs	703.72	Joback Method

Sources

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=C58516555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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