2-Ethylbutyric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C12H14Cl2O2/c1-3-8(4-2)12(15)16-9-5-6-10(13)11(14)7-9/h5-8H,3-4H2,1-2H3
InchiKey: SBLSKPMQKSFBRL-UHFFFAOYSA-N
Formula: C12H14Cl2O2
SMILES: CCC(CC)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 261.14

Physical Properties

Property code	Value	Unit	Source
gf	-116.91	kJ/mol	Joback Method
hf	-358.98	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.335		Crippen Method
mcvol	188.100	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	661.31	K	Joback Method
tc	880.74	K	Joback Method
tf	393.46	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.80	J/mol×K	661.31	Joback Method
cpg	504.46	J/mol×K	844.17	Joback Method
cpg	494.53	J/mol×K	807.59	Joback Method
cpg	483.81	J/mol×K	771.02	Joback Method
cpg	472.30	J/mol×K	734.45	Joback Method
cpg	459.97	J/mol×K	697.88	Joback Method
cpg	513.62	J/mol×K	880.74	Joback Method
dvisc	0.0001486	Pa×s	661.31	Joback Method

dvisc	0.0001874	Pa×s	616.67	Joback Method
dvisc	0.0002451	Pa×s	572.03	Joback Method
dvisc	0.0003354	Pa×s	527.38	Joback Method
dvisc	0.0004865	Pa×s	482.74	Joback Method
dvisc	0.0007610	Pa×s	438.10	Joback Method
dvisc	0.0013178	Pa×s	393.46	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=U357756&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