2-Ethylbutyric acid, 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C13H17ClO2/c1-4-10(5-2)13(15)16-12-8-9(3)6-7-11(12)14/h6-8,10H,4-5H2,1-3

InchiKey: AXHQLGNAROZOLY-UHFFFAOYSA-N

Formula: C13H17ClO2

SMILES: CCC(CC)C(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-96.56	kJ/mol	Joback Method
hf	-363.88	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.990		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	646.76	K	Joback Method
tc	859.26	K	Joback Method
tf	374.81	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.14	J/mol×K	646.76	Joback Method
cpg	485.89	J/mol×K	682.18	Joback Method
cpg	499.79	J/mol×K	717.59	Joback Method
cpg	512.83	J/mol×K	753.01	Joback Method
cpg	525.05	J/mol×K	788.43	Joback Method
cpg	536.46	J/mol×K	823.84	Joback Method
cpg	547.07	J/mol×K	859.26	Joback Method
dvisc	0.0014216	Pa×s	374.81	Joback Method

dvisc	0.0007896	Pa×s	420.13	Joback Method
dvisc	0.0004918	Pa×s	465.46	Joback Method
dvisc	0.0003332	Pa×s	510.78	Joback Method
dvisc	0.0002405	Pa×s	556.11	Joback Method
dvisc	0.0001823	Pa×s	601.43	Joback Method
dvisc	0.0001437	Pa×s	646.76	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=U370469&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