2-Ethylbutyric acid, 2-formylphenyl ester

Inchi: InChI=1S/C13H16O3/c1-3-10(4-2)13(15)16-12-8-6-5-7-11(12)9-14/h5-10H,3-4H2,1-2H3
InchiKey: NWJRTMIRMYQPJQ-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: CCC(CC)C(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-174.52	kJ/mol	Joback Method
hf	-422.25	kJ/mol	Joback Method
hfus	24.63	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.841		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1637.00		NIST Webbook
tb	653.01	K	Joback Method
tc	863.44	K	Joback Method
tf	374.37	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.71	J/mol×K	653.01	Joback Method
cpg	476.91	J/mol×K	688.08	Joback Method
cpg	490.24	J/mol×K	723.15	Joback Method
cpg	502.73	J/mol×K	758.22	Joback Method
cpg	514.38	J/mol×K	793.30	Joback Method
cpg	525.23	J/mol×K	828.37	Joback Method
cpg	535.28	J/mol×K	863.44	Joback Method
dvisc	0.0019526	Pa×s	374.37	Joback Method
dvisc	0.0010467	Pa×s	420.81	Joback Method

dvisc	0.0006351	Pa×s	467.25	Joback Method
dvisc	0.0004218	Pa×s	513.69	Joback Method
dvisc	0.0002998	Pa×s	560.13	Joback Method
dvisc	0.0002245	Pa×s	606.57	Joback Method
dvisc	0.0001752	Pa×s	653.01	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=U369964&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