2-Ethylbutyric acid, 4-cyanophenyl ester

Inchi: InChI=1S/C13H15NO2/c1-3-11(4-2)13(15)16-12-7-5-10(9-14)6-8-12/h5-8,11H,3-4H2,1-2
InchiKey: MIGWVIXXPPCHLV-UHFFFAOYSA-N
Formula: C13H15NO2
SMILES: CCC(CC)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 217.26

Physical Properties

Property code	Value	Unit	Source
gf	58.18	kJ/mol	Joback Method
hf	-171.79	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.900		Crippen Method
mcvol	179.090	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1682.00		NIST Webbook
tb	706.43	K	Joback Method
tc	927.18	K	Joback Method
tf	397.36	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.04	J/mol×K	706.43	Joback Method
cpg	485.12	J/mol×K	743.22	Joback Method
cpg	497.31	J/mol×K	780.01	Joback Method
cpg	508.64	J/mol×K	816.81	Joback Method
cpg	519.13	J/mol×K	853.60	Joback Method
cpg	528.80	J/mol×K	890.39	Joback Method
cpg	537.67	J/mol×K	927.18	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=U369611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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