Ethyl 2-cyano-3-phenyl pentanoate

Inchi: InChI=1S/C14H17NO2/c1-3-12(11-8-6-5-7-9-11)13(10-15)14(16)17-4-2/h5-9,12-13H,3-4
InchiKey: AYJQJWSAESSXPI-UHFFFAOYSA-N
Formula: C14H17NO2
SMILES: CCOC(=O)C(C#N)C(CC)c1ccccc1
Mol. weight [g/mol]: 231.29
CAS: 20621-70-9

Physical Properties

Property code	Value	Unit	Source
gf	73.79	kJ/mol	Joback Method
hf	-186.24	kJ/mol	Joback Method
hfus	23.30	kJ/mol	Joback Method
hvap	67.89	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.883		Crippen Method
mcvol	193.180	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	723.89	K	Joback Method
tc	944.25	K	Joback Method
tf	381.11	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.04	J/mol×K	723.89	Joback Method
cpg	539.97	J/mol×K	760.62	Joback Method
cpg	552.91	J/mol×K	797.34	Joback Method
cpg	564.91	J/mol×K	834.07	Joback Method
cpg	575.99	J/mol×K	870.80	Joback Method
cpg	586.18	J/mol×K	907.52	Joback Method
cpg	595.53	J/mol×K	944.25	Joback Method

Sources

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=C20621709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume