3-CN-C6H4-COOCH3

Inchi: InChI=1S/C9H7NO2/c1-12-9(11)8-4-2-3-7(5-8)6-10/h2-5H,1H3
InchiKey: XPBHWSMZTSSEJE-UHFFFAOYSA-N
Formula: C9H7NO2
SMILES: COC(=O)c1cccc(C#N)c1
Mol. weight [g/mol]: 161.16
CAS: 13531-48-1

Physical Properties

Property code	Value	Unit	Source
affp	817.40	kJ/mol	NIST Webbook
basg	786.50	kJ/mol	NIST Webbook
ea	0.77 ± 0.09	eV	NIST Webbook
gf	26.94	kJ/mol	Joback Method
hf	-83.95	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	58.20	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.345		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	615.35	K	Joback Method
tc	848.48	K	Joback Method
tf	367.28	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.21	J/mol×K	615.35	Joback Method
cpg	286.09	J/mol×K	654.20	Joback Method
cpg	295.30	J/mol×K	693.06	Joback Method
cpg	303.87	J/mol×K	731.91	Joback Method
cpg	311.80	J/mol×K	770.77	Joback Method
cpg	319.10	J/mol×K	809.62	Joback Method

cpg	325.78	J/mol×K	848.48	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=C13531481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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