Benzoic acid, 4-cyano-, methyl ester

Other names:	Benzoic acid, p-cyano-, methyl ester
	p-Cyanobenzoic acid methyl ester
	Methyl p-cyanobenzoate
	Methyl 4-cyanobenzoate
	4-Cyanobenzoic acid methyl ester
Inchi:	InChI=1S/C9H7NO2/c1-12-9(11)8-4-2-7(6-10)3-5-8/h2-5H,1H3
InchiKey:	KKZMIDYKRKGJHG-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	COC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]:	161.16
CAS:	1129-35-7

Physical Properties

Property code	Value	Unit	Source
affp	816.60	kJ/mol	NIST Webbook
basg	785.60	kJ/mol	NIST Webbook
ea	0.85 ± 0.09	eV	NIST Webbook
ea	0.98 ± 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
ie	9.72	eV	NIST Webbook
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	1.60	NIST Webbook

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=C1129357&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume