3-ACETYLBENZONITRILE

Other names:	1-(3-cyanophenyl)ethanone
	3'-Cyanoacetophenone
	3-CN-C6H4-COCH3
	Benzonitrile, 3-acetyl-
	m-acetylbenzonitrile
	m-cyanoacetophenone
Inchi:	InChI=1S/C9H7NO/c1-7(11)9-4-2-3-8(5-9)6-10/h2-5H,1H3
InchiKey:	SBCFGFDAZCTSRH-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	CC(=O)c1cccc(C#N)c1
Mol. weight [g/mol]:	145.16

Physical Properties

Property code	Value	Unit	Source
af	0.4832		Cheméo Relay (1.0)
affp	827.20	kJ/mol	NIST Webbook
basg	795.40	kJ/mol	NIST Webbook
gf	131.94	kJ/mol	Joback Method
hf	46.91	kJ/mol	Cheméo Relay (1.0)
hfus	15.82	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-1.98		Cheméo Relay (1.0)
logp	1.761		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	536.19	K	Cheméo Relay (1.0)
tc	782.55	K	Cheméo Relay (1.0)
tf	329.70	K	Cheméo Relay (1.0)
vc	0.430	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	254.59	J/mol×K	592.93	Joback Method
cpg	264.55	J/mol×K	632.36	Joback Method
cpg	273.81	J/mol×K	671.79	Joback Method
cpg	282.40	J/mol×K	711.22	Joback Method
cpg	290.34	J/mol×K	750.65	Joback Method
cpg	297.67	J/mol×K	790.09	Joback Method
cpg	304.42	J/mol×K	829.52	Joback Method
hvapt	94.70	kJ/mol	298.15	Thermochemical study of the isomeric compounds: 3-acetylbenzonitrile and benzoylacetonitrile

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical study of the isomeric compounds: 3-acetylbenzonitrile and benzoylacetonitrile:	https://www.doi.org/10.1016/j.jct.2015.08.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6136681&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume