Benzenepropanenitrile, «beta»-oxo-

Other names:	.alpha.-cyanoacetophenone
	.beta.-oxobenzenepropanenitrile
	.omega.-cyanoacetophenone
	2-Cyanoacetyl phenone
	2-cyanoacetophenone
	3-Phenyl-3-oxopropanenitrile
	3-oxo-3-phenylpropanenitrile
	3-phenyl-3-ketopropionitrile
	Acetonitrile, benzoyl-
	Acetophenone, 2-cyano-
	Cyanoacetophenone
	Hydrocinnamonitrile, «beta»-oxo-
	NSC 4713
	benzenepropanenitrile, .beta.-oxo-
	benzoylacetonitrile
	benzoylcyanomethane
	cyanomethyl phenyl ketone
	phenacyl cyanide
	«alpha»-Cyanoacetophenone
	«omega»-Cyanoacetophenone
Inchi:	InChI=1S/C9H7NO/c10-7-6-9(11)8-4-2-1-3-5-8/h1-5H,6H2
InchiKey:	ZJRCIQAMTAINCB-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	N#CCC(=O)c1ccccc1
Mol. weight [g/mol]:	145.16
CAS:	614-16-4

Physical Properties

Property code	Value	Unit	Source
chs	-4549.70	kJ/mol	NIST Webbook
chs	-4519.72 ± 0.42	kJ/mol	NIST Webbook
gf	141.57	kJ/mol	Joback Method
hf	70.12	kJ/mol	NIST Webbook
hfs	7.50	kJ/mol	NIST Webbook
hfs	-22.30 ± 0.42	kJ/mol	NIST Webbook
hfus	16.21	kJ/mol	Joback Method
hsub	92.50	kJ/mol	NIST Webbook

hvap	55.13	kJ/mol	Joback Method
ie	9.56 ± 0.05	eV	NIST Webbook
log10ws	-2.42		Crippen Method
logp	1.783		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	587.95	K	Joback Method
tc	823.51	K	Joback Method
tf	332.53	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.84	J/mol×K	587.95	Joback Method
cpg	266.07	J/mol×K	627.21	Joback Method
cpg	275.54	J/mol×K	666.47	Joback Method
cpg	284.28	J/mol×K	705.73	Joback Method
cpg	292.34	J/mol×K	744.99	Joback Method
cpg	299.75	J/mol×K	784.25	Joback Method
cpg	306.55	J/mol×K	823.51	Joback Method
hsubt	99.80	kJ/mol	325.50	NIST Webbook
hvapt	98.50	kJ/mol	298.15	Thermochemical study of the isomeric compounds: 3-acetylbenzonitrile and benzoylacetonitrile

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	1.30	NIST Webbook

Sources

Thermochemical study of the isomeric compounds: 3-acetylbenzonitrile and benzoylacetonitrile:	https://www.doi.org/10.1016/j.jct.2015.08.008
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=C614164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume