Benzeneacetonitrile, «alpha»-oxo-

Other names:	Glyoxylonitrile, phenyl- «alpha»-Oxobenzeneacetonitrile «alpha»-Tolunitrile, «alpha»-oxo- Benzoyl cyanide Benzoyl nitrile Phenylglyoxylonitrile
Inchi:	InChI=1S/C8H5NO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H
InchiKey:	GJQBHOAJJGIPRH-UHFFFAOYSA-N
Formula:	C8H5NO
SMILES:	N#CC(=O)c1ccccc1
Mol. weight [g/mol]:	131.13
CAS:	613-90-1

Physical Properties

Property code	Value	Unit	Source
chs	-3901.50 ± 0.30	kJ/mol	NIST Webbook
chs	-3936.00	kJ/mol	NIST Webbook
ea	1.13 ± 0.09	eV	NIST Webbook
gf	133.15	kJ/mol	Joback Method
hf	117.50	kJ/mol	NIST Webbook
hfs	38.90 ± 0.30	kJ/mol	NIST Webbook
hfs	73.20	kJ/mol	NIST Webbook
hfus	13.62	kJ/mol	Joback Method
hsub	78.70	kJ/mol	NIST Webbook
hsub	78.70 ± 4.20	kJ/mol	NIST Webbook
hvap	52.90	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.393		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	479.20	K	NIST Webbook
tc	805.54	K	Joback Method
tf	321.26	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.96	J/mol×K	565.07	Joback Method
cpg	221.12	J/mol×K	605.15	Joback Method
cpg	229.57	J/mol×K	645.23	Joback Method
cpg	237.35	J/mol×K	685.31	Joback Method
cpg	244.48	J/mol×K	725.38	Joback Method
cpg	251.01	J/mol×K	765.46	Joback Method
cpg	256.98	J/mol×K	805.54	Joback Method
hvapt	52.00	kJ/mol	399.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C613901&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
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
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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

Latest version available from:
https://www.chemeo.com/cid/24-242-6/Benzeneacetonitrile-alpha-oxo.pdf
Generated by Cheméo on 2025-12-23 09:49:22.974750642 +0000 UTC m=+6231560.504791312.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.