

Benzeneacetonitrile, «alpha»-hydroxy-

Other names:	Benzaldehyde, cyanohydrin «alpha»-Cyanobenzyl alcohol «alpha»-Hydroxybenzeneacetonitrile Mandelic acid nitrile Mandelonitrile Phenylglycolonitrile Acetonitrile, hydroxyphenyl- Amygdalonitrile Benzaldehydkyanhydrin Glycolonitrile, phenyl- Nitril kyseliny mandlove (.+/-.)-Mandelonitrile NSC 77668 Hydroxybenzyl cyanide
Inchi:	InChI=1S/C8H7NO/c9-6-8(10)7-4-2-1-3-5-7/h1-5,8,10H
InchiKey:	NNICRUQPODTGRU-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	N#CC(O)c1ccccc1
Mol. weight [g/mol]:	133.15
CAS:	532-28-5

Physical Properties

Property code	Value	Unit	Source
gf	122.81	kJ/mol	Joback Method
hf	35.45	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	62.45	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.244		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	443.20	K	NIST Webbook
tc	821.02	K	Joback Method
tf	317.15	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.83	J/mol×K	602.94	Joback Method
cpg	251.44	J/mol×K	639.29	Joback Method
cpg	259.44	J/mol×K	675.63	Joback Method
cpg	266.87	J/mol×K	711.98	Joback Method
cpg	273.75	J/mol×K	748.33	Joback Method
cpg	280.13	J/mol×K	784.67	Joback Method
cpg	286.03	J/mol×K	821.02	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=C532285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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

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