

O-BENZYLHYDROXYLAMINE

Other names:	(Benzyloxy)amine Hydroxylamine, O-benzyl- O-Benzylhydroxylamine Snr 1635
Inchi:	InChI=1S/C7H9NO/c8-9-6-7-4-2-1-3-5-7/h1-5H,6,8H2
InchiKey:	XYEOALKITRFCJJ-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	NOCc1ccccc1
Mol. weight [g/mol]:	123.15

Physical Properties

Property code	Value	Unit	Source
af	0.4756		Cheméo Relay (1.0)
gf	81.92	kJ/mol	Joback Method
hf	94.15	kJ/mol	Cheméo Relay (1.0)
hfus	14.31	kJ/mol	Joback Method
hvap	53.80	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-0.81		Cheméo Relay (1.0)
logp	1.077		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	467.74	K	Cheméo Relay (1.0)
tc	701.53	K	Cheméo Relay (1.0)
tf	284.00	K	Cheméo Relay (1.0)
vc	0.357	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.60	J/mol×K	481.19	Joback Method
cpg	221.14	J/mol×K	518.59	Joback Method
cpg	232.01	J/mol×K	555.99	Joback Method
cpg	242.23	J/mol×K	593.39	Joback Method

cpg	251.83	J/mol×K	630.79	Joback Method
cpg	260.82	J/mol×K	668.19	Joback Method
cpg	269.21	J/mol×K	705.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.50 ± 0.50	K	4.00	NIST Webbook
tbrp	363.00	K	2.00	NIST Webbook

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622333&Units=SI

Legend

af:	Acentric Factor
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
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

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