Benzyl isocyanate

Other names: Benzene, (isocyanatomethyl)-
Inchi: InChI=1S/C8H7NO/c10-7-9-6-8-4-2-1-3-5-8/h1-5H,6H2
InchiKey: YDNLNVZZTACNJX-UHFFFAOYSA-N
Formula: C8H7NO
SMILES: O=C=NCc1ccccc1
Mol. weight [g/mol]: 133.15
CAS: 3173-56-6

Physical Properties

Property code	Value	Unit	Source
hf	22.67	kJ/mol	Joback Method
hvap	45.21	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	1.522		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1125.80		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	475.79	K	Joback Method
tc	696.70	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	42.30	kJ/mol	363.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3173566&Units=SI

Legend

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature