2-METHYL-BENZOOXAZOLE

Other names:	2-Methylbenzoxazol
	2-Methylbenzoxazole
	USAF ek-982
Inchi:	InChI=1S/C8H7NO/c1-6-9-7-4-2-3-5-8(7)10-6/h2-5H,1H3
InchiKey:	DQSHFKPKFISSNM-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	Cc1nc2ccccc2o1
Mol. weight [g/mol]:	133.15

Physical Properties

Property code	Value	Unit	Source
hf	-23.53	kJ/mol	Cheméo Relay (1.0)
logp	2.136		Crippen Method
mcvol	100.510	ml/mol	McGowan Method
tb	451.20	K	NIST Webbook
tb	473.70	K	NIST Webbook
tf	273.70	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.70	K	1.60	NIST Webbook

Sources

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=C95216&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point