

exo-2-Norbornyl isothiocyanate

Other names:	exo-bicyclo[2.2.1]hept-2-yl isothiocyanate
Inchi:	InChI=1S/C8H11NS/c10-5-9-8-4-6-1-2-7(8)3-6/h6-8H,1-4H2
InchiKey:	RBGDFYZLQKZUCO-UHFFFAOYSA-N
Formula:	C8H11NS
SMILES:	S=C=NC1CC2CCC1C2
Mol. weight [g/mol]:	153.25

Physical Properties

Property code	Value	Unit	Source
logp	2.278		Crippen Method
mcvol	119.590	ml/mol	McGowan Method

Sources

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=C18530331&Units=SI
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

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/40-666-8/exo-2-Norbornyl-isothiocyanate.pdf>

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