

Bicyclo[2.2.1]heptane, 2-isothiocyanato-, exo-

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
CAS:	18530-33-1

Physical Properties

Property code	Value	Unit	Source
hf	194.72	kJ/mol	Joback Method
hvap	43.53	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.278		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	541.47	K	Joback Method
tc	792.87	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18530331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

hf:	Enthalpy of formation 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

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