

3-Bromopropyl isothiocyanate

Inchi:	InChI=1S/C4H6BrNS/c5-2-1-3-6-4-7/h1-3H2
InchiKey:	RIUVKCFFZBZEHS-UHFFFAOYSA-N
Formula:	C4H6BrNS
SMILES:	S=C=NCCCBBr
Mol. weight [g/mol]:	180.07
CAS:	2799-73-7

Physical Properties

Property code	Value	Unit	Source
hf	184.51	kJ/mol	Joback Method
hvap	41.37	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.874		Crippen Method
mcvol	102.450	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	503.03	K	Joback Method
tc	741.88	K	Joback Method

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=C2799737&Units=SI

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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