2,3-Dibromopropyl isothiocyanate

Inchi: InChI=1S/C4H5Br2NS/c5-1-4(6)2-7-3-8/h4H,1-2H2
InchiKey: AFQQAAKQKFCSPQ-UHFFFAOYSA-N
Formula: C4H5Br2NS
SMILES: S=C=NCC(Br)CBr
Mol. weight [g/mol]: 258.96
CAS: 51784-10-2

Physical Properties

Property code	Value	Unit	Source
hf	205.56	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.248		Crippen Method
mcvol	119.950	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
tb	568.75	K	Joback Method
tc	829.11	K	Joback Method

Sources

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=C51784102&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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