

2-Bromoethyl isothiocyanate

Inchi: InChI=1S/C3H4BrNS/c4-1-2-5-3-6/h1-2H2
InchiKey: SGJVENMTWFTZOJ-UHFFFAOYSA-N
Formula: C3H4BrNS
SMILES: S=C=NCCBr
Mol. weight [g/mol]: 166.04
CAS: 1483-41-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 205.15 | kJ/mol | Joback Method |
| hvap | 39.15 | kJ/mol | Joback Method |
| log10ws | -1.44 | | Crippen Method |
| logp | 1.484 | | Crippen Method |
| mcvol | 88.360 | ml/mol | McGowan Method |
| pc | 4994.44 | kPa | Joback Method |
| tb | 480.15 | K | Joback Method |
| tc | 723.54 | K | Joback Method |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1483416&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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