

«alpha»-Isothiocyanato-«gamma»-butyrolactone

Inchi: InChI=1S/C5H5NO2S/c7-5-4(6-3-9)1-2-8-5/h4H,1-2H2
InchiKey: MSBPBCHCQJBHNC-UHFFFAOYSA-N
Formula: C5H5NO2S
SMILES: O=C1OCCC1N=C=S
Mol. weight [g/mol]: 143.16
CAS: 61315-63-7

Physical Properties

Property code	Value	Unit	Source
hf	-71.68	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.405		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
tb	569.80	K	Joback Method
tc	839.98	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=C61315637&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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