

N-Allyl O-ethyl thiocarbamate

Inchi: InChI=1S/C6H11NOS/c1-3-5-7-6(9)8-4-2/h3H,1,4-5H2,2H3,(H,7,9)
InchiKey: ZRPRNLNEYWYWLO-UHFFFAOYSA-N
Formula: C6H11NOS
SMILES: C=CCN=C(S)OCC
Mol. weight [g/mol]: 145.22
CAS: 817-97-0

Physical Properties

Property code	Value	Unit	Source
hf	-63.05	kJ/mol	Joback Method
hvap	40.82	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.495		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	495.20	K	Joback Method
tc	712.73	K	Joback Method

Sources

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=C817970&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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