

3-Methylhexyl isothiocyanate

Inchi: InChI=1S/C8H15NS/c1-3-4-8(2)5-6-9-7-10/h8H,3-6H2,1-2H3
InchiKey: TXKNVIMTEJTWJQ-UHFFFAOYSA-N
Formula: C8H15NS
SMILES: CCCC(C)CCN=C=S
Mol. weight [g/mol]: 157.28
CAS: 206761-72-0

Physical Properties

Property code	Value	Unit	Source
hf	70.34	kJ/mol	Joback Method
hvap	43.45	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.916		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	527.95	K	Joback Method
tc	740.54	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C206761720&Units=SI>
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>

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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