

3-(Diethylamino)propyl isothiocyanate

Inchi:	InChI=1S/C8H16N2S/c1-3-10(4-2)7-5-6-9-8-11/h3-7H2,1-2H3
InchiKey:	QPBVKSLJBRCKIF-UHFFFAOYSA-N
Formula:	C8H16N2S
SMILES:	CCN(CC)CCCN=C=S
Mol. weight [g/mol]:	172.29
CAS:	2626-52-0

Physical Properties

Property code	Value	Unit	Source
hf	143.15	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.821		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
tb	540.83	K	Joback Method
tc	745.91	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=C2626520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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