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/ci990307l
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