Methyl isothiocyanate

Inchi: InChI=1S/C2H3NS/c1-3-2-4/h1H3
InchiKey: LGDSHSYDSCRFAB-UHFFFAOYSA-N
Formula: C2H3NS
SMILES: CN=C=S
Mol. weight [g/mol]: 73.12
CAS: 556-61-6

Physical Properties

Property code	Value	Unit	Source
hf	199.46	kJ/mol	Joback Method
hvap	30.49	kJ/mol	Joback Method
log10ws	-1.00		Aqueous Solubility Prediction Method
logp	0.719		Crippen Method
mcvol	56.770	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
rinpol	742.00		NIST Webbook
tb	391.11	K	Joback Method
tc	617.59	K	Joback Method
tf	307.48	K	Aqueous Solubility Prediction Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51778e+01
Coeff. B	-3.90615e+03
Coeff. C	-2.22300e+01
Temperature range (K), min.	284.56
Temperature range (K), max.	418.14

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U290251&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point