4-Methylpentyl isothiocyanate

Inchi: InChI=1S/C7H13NS/c1-7(2)4-3-5-8-6-9/h7H,3-5H2,1-2H3
InchiKey: CZWUENKYXFGDIG-UHFFFAOYSA-N
Formula: C7H13NS
SMILES: CC(C)CCCN=C=S
Mol. weight [g/mol]: 143.25
CAS: 17608-07-0

Physical Properties

Property code	Value	Unit	Source
hf	90.98	kJ/mol	Joback Method
hvap	41.23	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.525		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1136.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1162.30		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1162.30		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	505.07	K	Joback Method
tc	721.13	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17608070&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature