Crotonyl isothiocyanate

Inchi: InChI=1S/C5H5NOS/c1-2-3-5(7)6-4-8/h2-3H,1H3/b3-2+
InchiKey: GGYYXENTGJDZTN-NSCUHMNNSA-N
Formula: C5H5NOS
SMILES: CC=CC(=O)N=C=S
Mol. weight [g/mol]: 127.16
CAS: 60034-28-8

Physical Properties

Property code	Value	Unit	Source
hf	142.18	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.192		Crippen Method
mcvol	96.310	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	517.78	K	Joback Method
tc	757.13	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60034288&Units=SI

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