1,4-Butane diisothiocyanate

Inchi: InChI=1S/C6H8N2S2/c9-5-7-3-1-2-4-8-6-10/h1-4H2
InchiKey: RRSISCMPUAGVJN-UHFFFAOYSA-N
Formula: C6H8N2S2
SMILES: S=C=NCCCCN=C=S
Mol. weight [g/mol]: 172.27
CAS: 4430-51-7

Physical Properties

Property code	Value	Unit	Source
hf	400.97	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.972		Crippen Method
mcvol	130.860	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	628.58	K	Joback Method
tc	885.40	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=C4430517&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