

berteroin

Other names:	5-(Methylthio)pentyl isothiocyanate
Inchi:	InChI=1S/C7H13NS2/c1-10-6-4-2-3-5-8-7-9/h2-6H2,1H3
InchiKey:	HBVIMVJTUQNSEP-UHFFFAOYSA-N
Formula:	C7H13NS2
SMILES:	CSCCCCCC(S)=NO
Mol. weight [g/mol]:	175.31
CAS:	4430-42-6

Physical Properties

Property code	Value	Unit	Source
hf	-187.26	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.627		Crippen Method
mcvol	153.740	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1552.80		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1552.80		NIST Webbook
rinpol	1503.00		NIST Webbook
ripol	2242.00		NIST Webbook
tb	659.94	K	Joback Method
tc	873.51	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4430426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
rip_{ol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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