

1-Butene, 4-isothiocyanato-

Other names:	1-butene 4-isothiocyanate 3-Butenyl isothiocyanate 4-Isothiocyanato-1-butene But-3-enyl isothiocyanate Isothiocyanic acid, 3-butenyl ester
Inchi:	InChI=1S/C5H7NS/c1-2-3-4-6-5-7/h2H,1,3-4H2
InchiKey:	SKIHGKNFJKJXPX-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	C=CCCN=C=S
Mol. weight [g/mol]:	113.18
CAS:	3386-97-8

Physical Properties

Property code	Value	Unit	Source
hf	262.97	kJ/mol	Joback Method
hvap	36.49	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.665		Crippen Method
mcvol	94.740	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	982.60		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	982.60		NIST Webbook
rinpol	984.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1403.00		NIST Webbook

ripol	1403.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1463.00		NIST Webbook
tb	456.43	K	Joback Method
tc	679.19	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.20	kJ/mol	392.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.69539e+01
Coeff. B	-5.43410e+03
Temperature range (K), min.	326.05
Temperature range (K), max.	466.75

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3386978&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/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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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