

3-Vinyl-1,2-dithiacyclohex-5-ene

Other names:	1,2-Dithi-5-ene, 3-ethenyl 3,4-Dihydro-3-vinyl-1,2-dithiin 3-Ethenyl-1,2-dithi-5-ene 3-Vinyl-1,2-dithi-5-ene 3-Vinyl-4H-1,2-dithiin 4H-1,2-Dithiin, 3-ethenyl 3-Vinyl-1,2-dithiocyclohex-5-ene
Inchi:	InChI=1S/C6H8S2/c1-2-6-4-3-5-7-8-6/h2-3,5-6H,1,4H2
InchiKey:	NLHCAGKOLUBCBZ-UHFFFAOYSA-N
Formula:	C6H8S2
SMILES:	C=CC1CC=CSS1
Mol. weight [g/mol]:	144.26
CAS:	62488-53-3

Physical Properties

Property code	Value	Unit	Source
gf	221.61	kJ/mol	Joback Method
hf	160.88	kJ/mol	Joback Method
hfus	10.39	kJ/mol	Joback Method
hvap	40.62	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.840		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook

ripol	1761.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1760.00		NIST Webbook
tb	447.73	K	Joback Method
tc	695.41	K	Joback Method
tf	330.66	K	Joback Method
vc	0.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.06	J/mol×K	447.73	Joback Method
cpg	207.13	J/mol×K	489.01	Joback Method
cpg	219.27	J/mol×K	530.29	Joback Method
cpg	230.54	J/mol×K	571.57	Joback Method
cpg	240.97	J/mol×K	612.85	Joback Method
cpg	250.62	J/mol×K	654.13	Joback Method
cpg	259.53	J/mol×K	695.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62488533&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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