

4H-1,3-Dithiin, 4-methyl-2-(1-propenyl)-

Other names:	4-Methyl-2-propenyl-4H-[1,3]dithiine
Inchi:	InChI=1S/C8H12S2/c1-3-4-8-9-6-5-7(2)10-8/h3-8H,1-2H3/b4-3+
InchiKey:	ALDAFTNRTWJFQH-ONEGZZNKSA-N
Formula:	C8H12S2
SMILES:	CC=CC1SC=CC(C)S1
Mol. weight [g/mol]:	172.31
CAS:	60051-35-6

Physical Properties

Property code	Value	Unit	Source
gf	223.12	kJ/mol	Joback Method
hf	91.05	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	45.40	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.271		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1331.00		NIST Webbook
rinpol	1331.00		NIST Webbook
tb	496.30	K	Joback Method
tc	741.38	K	Joback Method
tf	345.64	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.26	J/molxK	496.30	Joback Method
cpg	294.45	J/molxK	537.15	Joback Method
cpg	309.55	J/molxK	577.99	Joback Method
cpg	323.60	J/molxK	618.84	Joback Method
cpg	336.67	J/molxK	659.69	Joback Method
cpg	348.81	J/molxK	700.53	Joback Method

Sources

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=C60051356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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