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

Other names: 4-Methyl-3-propenyl-3,4-dihydro-[1,2]dithiine
Inchi: InChI=1S/C8H12S2/c1-3-4-8-7(2)5-6-9-10-8/h3-8H,1-2H3/b4-3+
InchiKey: GKMUSNHMVCWOHG-ONEGZZNKSA-N
Formula: C8H12S2
SMILES: CC=CC1SSC=CC1C
Mol. weight [g/mol]: 172.31
CAS: 60051-36-7

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	-3.90		Crippen Method
logp	3.476		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1332.00		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/mol×K	496.30	Joback Method
cpg	294.45	J/mol×K	537.15	Joback Method
cpg	309.55	J/mol×K	577.99	Joback Method
cpg	323.60	J/mol×K	618.84	Joback Method
cpg	336.67	J/mol×K	659.69	Joback Method

cpg	348.81	J/mol×K	700.53	Joback Method
cpg	360.07	J/mol×K	741.38	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=C60051367&Units=SI

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