4-Vinyl-4H-1,3-dithiin

Inchi: InChI=1S/C6H8S2/c1-2-6-3-4-7-5-8-6/h2-4,6H,1,5H2
InchiKey: AHVUAKSNJFPTNT-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: C=CC1C=CSCS1
Mol. weight [g/mol]: 144.26

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	-2.81		Crippen Method
logp	2.492		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
tb	447.73	K	Joback Method
tc	695.41	K	Joback Method
tf	330.66	K	Joback Method
vc	0.363	m3/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=R612263&Units=SI
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

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