2-Vinyl-1,3-dithiane

Other names: 1,3-Dithiane, 2-ethenyl
Inchi: InChI=1S/C6H10S2/c1-2-6-7-4-3-5-8-6/h2,6H,1,3-5H2
InchiKey: SIZZLUKBSIWVMD-UHFFFAOYSA-N
Formula: C6H10S2
SMILES: C=CC1SCCCS1
Mol. weight [g/mol]: 146.27
CAS: 61685-40-3

Physical Properties

Property code	Value	Unit	Source
gf	191.65	kJ/mol	Joback Method
hf	103.10	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.369		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1679.00		NIST Webbook
tb	448.57	K	Joback Method
tc	693.51	K	Joback Method
tf	329.90	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.74	J/mol×K	448.57	Joback Method
cpg	223.33	J/mol×K	489.39	Joback Method
cpg	236.96	J/mol×K	530.22	Joback Method
cpg	249.67	J/mol×K	571.04	Joback Method
cpg	261.49	J/mol×K	611.86	Joback Method
cpg	272.48	J/mol×K	652.68	Joback Method
cpg	282.67	J/mol×K	693.51	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=C61685403&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume