1,2-Dithiacyclopent-3-ene

Inchi: InChI=1S/C3H4S2/c1-2-4-5-3-1/h1-2H,3H2
InchiKey: PCGDBWLKAYKBTN-UHFFFAOYSA-N
Formula: C3H4S2
SMILES: C1=CSSC1
Mol. weight [g/mol]: 104.19
CAS: 288-26-6

Physical Properties

Property code	Value	Unit	Source
gf	128.32	kJ/mol	Joback Method
hf	123.87	kJ/mol	Joback Method
hfus	4.93	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.895		Crippen Method
mcvol	70.670	ml/mol	McGowan Method
pc	6209.79	kPa	Joback Method
rinpol	945.00		NIST Webbook
rinpol	958.60		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	958.60		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	945.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	382.81	K	Joback Method
tc	625.27	K	Joback Method
tf	306.37	K	Joback Method
vc	0.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.43	J/mol×K	382.81	Joback Method
cpg	109.35	J/mol×K	423.22	Joback Method
cpg	116.60	J/mol×K	463.63	Joback Method
cpg	123.24	J/mol×K	504.04	Joback Method
cpg	129.31	J/mol×K	544.45	Joback Method
cpg	134.85	J/mol×K	584.86	Joback Method
cpg	139.91	J/mol×K	625.27	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=C288266&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