2-Methyl-1,3-dithiacyclopentane

Other names: 1,3-Dithiolane, 2-methyl-
2-Methyl-1,3-dithiolane
Inchi: InChI=1S/C4H8S2/c1-4-5-2-3-6-4/h4H,2-3H2,1H3
InchiKey: CARJCVDELAMAEJ-UHFFFAOYSA-N
Formula: C4H8S2
SMILES: CC1SCCS1
Mol. weight [g/mol]: 120.24
CAS: 5616-51-3

Physical Properties

Property code	Value	Unit	Source
gf	99.07	kJ/mol	Joback Method
hf	25.11	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	36.38	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.812		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	1438.00		NIST Webbook
tb	401.86	K	Joback Method
tc	638.04	K	Joback Method

tf	312.64	K	Joback Method
vc	0.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.32	J/mol×K	401.86	Joback Method
cpg	160.81	J/mol×K	441.22	Joback Method
cpg	171.57	J/mol×K	480.59	Joback Method
cpg	181.64	J/mol×K	519.95	Joback Method
cpg	191.04	J/mol×K	559.31	Joback Method
cpg	199.83	J/mol×K	598.68	Joback Method
cpg	208.02	J/mol×K	638.04	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=C5616513&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