4-methyl-1,2-dithiepane

Other names: 1,2-Dithiepane, 4-methyl
Inchi: InChI=1S/C6H12S2/c1-6-3-2-4-7-8-5-6/h6H,2-5H2,1H3
InchiKey: BTSPIBMKYWNUOV-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1CCCSSC1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	91.71	kJ/mol	Joback Method
hf	-28.49	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	41.18	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.798		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1231.00		NIST Webbook
tb	456.16	K	Joback Method
tc	705.33	K	Joback Method
tf	328.14	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.08	J/mol×K	456.16	Joback Method
cpg	240.57	J/mol×K	497.69	Joback Method
cpg	256.06	J/mol×K	539.22	Joback Method
cpg	270.59	J/mol×K	580.75	Joback Method
cpg	284.16	J/mol×K	622.27	Joback Method

cpg	296.82	J/mol×K	663.80	Joback Method
cpg	308.58	J/mol×K	705.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82348&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

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