1,2-Dithiepane

Other names:	1,2-Dithiacycloheptane
Inchi:	InChI=1S/C5H10S2/c1-2-4-6-7-5-3-1/h1-5H2
InchiKey:	KUSGATRNQCYALG-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	C1CCSSCC1
Mol. weight [g/mol]:	134.26
CAS:	6008-51-1

Physical Properties

Property code	Value	Unit	Source
gf	91.00	kJ/mol	Joback Method
hf	12.49	kJ/mol	Joback Method
hfus	4.68	kJ/mol	Joback Method
hvap	39.26	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.552		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	1210.00		NIST Webbook
tb	437.95	K	Joback Method
tc	691.84	K	Joback Method
tf	321.11	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.67	J/mol×K	437.95	Joback Method
cpg	197.41	J/mol×K	480.26	Joback Method
cpg	211.19	J/mol×K	522.58	Joback Method
cpg	224.04	J/mol×K	564.89	Joback Method
cpg	235.99	J/mol×K	607.21	Joback Method
cpg	247.08	J/mol×K	649.52	Joback Method
cpg	257.34	J/mol×K	691.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6008511&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

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