1,4-dithiepane

Other names: 1,4-Dithiacycloheptane
1,5-Dithiepane
Inchi: InChI=1S/C5H10S2/c1-2-6-4-5-7-3-1/h1-5H2
InchiKey: DNWRQNQDWZNZEB-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: C1CSCCSC1
Mol. weight [g/mol]: 134.26

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	-1.58		Crippen Method
logp	1.857		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1113.00		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

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=R155225&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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