

1,2,5-Trithiepane

Other names:	1,2,5-Trithiapane
Inchi:	InChI=1S/C4H8S3/c1-3-6-7-4-2-5-1/h1-4H2
InchiKey:	JOAOASQIWYLMQC-UHFFFAOYSA-N
Formula:	C4H8S3
SMILES:	C1CSSCCS1
Mol. weight [g/mol]:	152.30
CAS:	6576-93-8

Physical Properties

Property code	Value	Unit	Source
gf	122.44	kJ/mol	Joback Method
hf	78.39	kJ/mol	Joback Method
hfus	5.75	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.115		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	462.90	K	Joback Method
tc	739.44	K	Joback Method
tf	393.29	K	Joback Method
vc	0.324	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.25	J/mol×K	462.90	Joback Method
cpg	197.42	J/mol×K	508.99	Joback Method
cpg	209.61	J/mol×K	555.08	Joback Method
cpg	220.85	J/mol×K	601.17	Joback Method
cpg	231.19	J/mol×K	647.26	Joback Method
cpg	240.67	J/mol×K	693.35	Joback Method
cpg	249.33	J/mol×K	739.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6576938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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