Thietane, 2-methyl-

Other names:	Butane, 1,3-epithio- «alpha»-Methylthietane 2-Methylthiacyclobutane 2-Methylthietane
Inchi:	InChI=1S/C4H8S/c1-4-2-3-5-4/h4H,2-3H2,1H3
InchiKey:	DUTRXPYVMIFJQZ-UHFFFAOYSA-N
Formula:	C4H8S
SMILES:	CC1CCS1
Mol. weight [g/mol]:	88.17
CAS:	17837-41-1

Physical Properties

Property code	Value	Unit	Source
gf	71.31	kJ/mol	Joback Method
hf	-13.99	kJ/mol	Joback Method
hfus	5.81	kJ/mol	Joback Method
hvap	30.40	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.512		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	723.00		NIST Webbook
rinpol	723.00		NIST Webbook
tb	349.76	K	Joback Method
tc	556.77	K	Joback Method
tf	232.71	K	Joback Method
vc	0.255	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.06	J/mol×K	349.76	Joback Method
cpg	122.49	J/mol×K	384.26	Joback Method
cpg	132.32	J/mol×K	418.76	Joback Method

cpg	141.57	J/mol×K	453.27	Joback Method
cpg	150.27	J/mol×K	487.77	Joback Method
cpg	158.45	J/mol×K	522.27	Joback Method
cpg	166.13	J/mol×K	556.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17837411&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