3,3-Dimethylthietane

Inchi: InChI=1S/C5H10S/c1-5(2)3-6-4-5/h3-4H2,1-2H3
InchiKey: RPRIYERFOHERFT-UHFFFAOYSA-N
Formula: C5H10S
SMILES: CC1(C)CSC1
Mol. weight [g/mol]: 102.20
CAS: 13188-85-7

Physical Properties

Property code	Value	Unit	Source
gf	74.24	kJ/mol	Joback Method
hf	-19.39	kJ/mol	Joback Method
hfus	2.10	kJ/mol	Joback Method
hvap	31.47	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.759		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
tb	372.88	K	Joback Method
tc	588.65	K	Joback Method
tf	267.88	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.95	J/mol×K	372.88	Joback Method
cpg	159.90	J/mol×K	408.84	Joback Method
cpg	171.69	J/mol×K	444.80	Joback Method
cpg	182.42	J/mol×K	480.76	Joback Method
cpg	192.22	J/mol×K	516.73	Joback Method
cpg	201.21	J/mol×K	552.69	Joback Method
cpg	209.49	J/mol×K	588.65	Joback Method

Sources

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=C13188857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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