

Thietane, 2,4-dimethyl-

Other names:	2,4-Dimethylthietane
Inchi:	InChI=1S/C5H10S/c1-4-3-5(2)6-4/h4-5H,3H2,1-2H3
InchiKey:	PCMVFKBBCXWSNV-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	CC1CC(C)S1
Mol. weight [g/mol]:	102.20
CAS:	43044-24-2

Physical Properties

Property code	Value	Unit	Source
gf	72.02	kJ/mol	Joback Method
hf	-54.97	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	32.31	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.900		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	367.97	K	Joback Method
tc	573.09	K	Joback Method
tf	239.74	K	Joback Method
vc	0.309	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.21	J/molxK	367.97	Joback Method
cpg	159.35	J/molxK	402.16	Joback Method
cpg	170.87	J/molxK	436.34	Joback Method
cpg	181.78	J/molxK	470.53	Joback Method
cpg	192.12	J/molxK	504.72	Joback Method
cpg	201.91	J/molxK	538.90	Joback Method
cpg	211.16	J/molxK	573.09	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=C43044242&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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