2,6-Dimethylthiane

Inchi: InChI=1S/C7H14S/c1-6-4-3-5-7(2)8-6/h6-7H,3-5H2,1-2H3
InchiKey: IHAMTZXWAMHHET-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CC1CCCC(C)S1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	64.66	kJ/mol	Joback Method
hf	-108.57	kJ/mol	Joback Method
hfus	10.45	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.680		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	957.00		NIST Webbook
rinpol	957.00		NIST Webbook
tb	422.27	K	Joback Method
tc	641.36	K	Joback Method
tf	255.24	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.70	J/mol×K	422.27	Joback Method
cpg	237.55	J/mol×K	458.78	Joback Method
cpg	253.57	J/mol×K	495.30	Joback Method
cpg	268.76	J/mol×K	531.81	Joback Method
cpg	283.14	J/mol×K	568.33	Joback Method
cpg	296.74	J/mol×K	604.84	Joback Method
cpg	309.57	J/mol×K	641.36	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=R535661&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

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