

2,4-DIMETHYLTETRAHYDROTHIOPHENE 1,1-DIOXIDE

Other names:	Dimethylsulfolane Thiophene, tetrahydro-2,4-dimethyl-, 1,1-dioxide DMS tetrahydro-2,4-dimethylthiophene 1,1-dioxide
Inchi:	InChI=1S/C6H12O2S/c1-5-3-6(2)9(7,8)4-5/h5-6H,3-4H2,1-2H3
InchiKey:	WKFQMDFSQFAIC-UHFFFAOYSA-N
Formula:	C6H12O2S
SMILES:	CC1CC(C)S(=O)(=O)C1
Mol. weight [g/mol]:	148.23

Physical Properties

Property code	Value	Unit	Source
hfus	17.21	kJ/mol	Joback Method
logp	0.830		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
tb	547.30	K	Cheméo Relay (1.0)
tf	317.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.30	J/mol×K	374.12	Joback Method
cpg	217.44	J/mol×K	404.44	Joback Method
cpg	231.01	J/mol×K	434.75	Joback Method
cpg	244.01	J/mol×K	465.07	Joback Method
cpg	256.44	J/mol×K	495.38	Joback Method
cpg	268.32	J/mol×K	525.70	Joback Method
cpg	279.66	J/mol×K	556.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003787&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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