5-methyl-dihydrofuran-2(3H)-thione

Inchi: InChI=1S/C5H6OS/c1-4-2-3-5(7)6-4/h2H,3H2,1H3
InchiKey: WFCOZOZWHFUXJU-UHFFFAOYSA-N
Formula: C5H6OS
SMILES: CC1=CCC(=S)O1
Mol. weight [g/mol]: 114.17

Physical Properties

Property code	Value	Unit	Source
gf	60.54	kJ/mol	Joback Method
hf	-36.30	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.638		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	5037.07	kPa	Joback Method
rinpol	1076.00		NIST Webbook
ripol	1877.00		NIST Webbook
tb	437.48	K	Joback Method
tc	665.99	K	Joback Method
tf	264.77	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.52	J/mol×K	437.48	Joback Method
cpg	158.11	J/mol×K	475.57	Joback Method
cpg	166.04	J/mol×K	513.65	Joback Method
cpg	173.37	J/mol×K	551.74	Joback Method
cpg	180.15	J/mol×K	589.82	Joback Method
cpg	186.42	J/mol×K	627.91	Joback Method
cpg	192.23	J/mol×K	665.99	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=R422510&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/37-973-1/5-methyl-dihydrofuran-2-3H-thione.pdf
Generated by Cheméo on 2024-04-17 20:30:28.087689597 +0000 UTC m=+15675077.008266912.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.