

2-Methyl-2,3-dihydrofuran-3-thiol

Inchi: InChI=1S/C5H8OS/c1-4-5(7)2-3-6-4/h2-5,7H,1H3
InchiKey: PZGLKZTWQCEEIT-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: CC1OC=CC1S
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-6.71	kJ/mol	Joback Method
hf	-142.13	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	38.21	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.217		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
tb	413.38	K	Joback Method
tc	641.07	K	Joback Method
tf	216.56	K	Joback Method
vc	0.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.40	J/mol×K	413.38	Joback Method
cpg	174.28	J/mol×K	451.33	Joback Method
cpg	185.49	J/mol×K	489.28	Joback Method
cpg	196.05	J/mol×K	527.22	Joback Method
cpg	205.97	J/mol×K	565.17	Joback Method
cpg	215.28	J/mol×K	603.12	Joback Method
cpg	224.00	J/mol×K	641.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R125823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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