Thiophene, 2-formyl-2,3-dihydro-

Other names: Thiophene, 2,3-dihydro-2-formyl
Inchi: InChI=1S/C5H6OS/c6-4-5-2-1-3-7-5/h1,3-5H,2H2
InchiKey: QWTALAUIEVWIGR-UHFFFAOYSA-N
Formula: C5H6OS
SMILES: O=CC1CC=CS1
Mol. weight [g/mol]: 114.17
CAS: 290354-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-1.93	kJ/mol	Joback Method
hf	-68.59	kJ/mol	Joback Method
hfus	9.81	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.204		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
tb	424.73	K	Joback Method
tc	649.92	K	Joback Method
tf	283.22	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.65	J/mol×K	424.73	Joback Method
cpg	159.76	J/mol×K	462.26	Joback Method
cpg	169.21	J/mol×K	499.79	Joback Method
cpg	178.01	J/mol×K	537.33	Joback Method
cpg	186.21	J/mol×K	574.86	Joback Method
cpg	193.83	J/mol×K	612.39	Joback Method

cpg	200.91	J/mol×K	649.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C290354700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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