2-Formyl-5-methyl-2,5-dihydrothiophene

Inchi: InChI=1S/C6H8OS/c1-5-2-3-6(4-7)8-5/h2-6H,1H3
InchiKey: SPJZOMMRMMVLLO-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC1C=CC(C=O)S1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
gf	-1.22	kJ/mol	Joback Method
hf	-109.57	kJ/mol	Joback Method
hfus	13.47	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.245		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	442.94	K	Joback Method
tc	664.66	K	Joback Method
tf	290.25	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.80	J/mol×K	442.94	Joback Method
cpg	200.62	J/mol×K	479.89	Joback Method
cpg	211.75	J/mol×K	516.85	Joback Method
cpg	222.20	J/mol×K	553.80	Joback Method
cpg	232.00	J/mol×K	590.75	Joback Method
cpg	241.19	J/mol×K	627.71	Joback Method
cpg	249.77	J/mol×K	664.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640312&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
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
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