2-formyl-5-methyl-4,5-dihydrothiophene

Inchi: InChI=1S/C6H8OS/c1-5-2-3-6(4-7)8-5/h3-5H,2H2,1H3
InchiKey: ZRBOFSXEZKEMKN-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC1CC=C(C=O)S1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
gf	-3.14	kJ/mol	Joback Method
hf	-100.70	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	42.69	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.595		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1734.00		NIST Webbook
tb	452.59	K	Joback Method
tc	676.09	K	Joback Method
tf	307.01	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.07	J/mol×K	452.59	Joback Method
cpg	199.06	J/mol×K	489.84	Joback Method
cpg	209.39	J/mol×K	527.09	Joback Method
cpg	219.10	J/mol×K	564.34	Joback Method
cpg	228.20	J/mol×K	601.59	Joback Method
cpg	236.72	J/mol×K	638.84	Joback Method
cpg	244.70	J/mol×K	676.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R169209&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume