3,4-Dimethyl-2,5-dihidrothiophene

Inchi: InChI=1S/C6H10S/c1-5-3-7-4-6(5)2/h3-4H2,1-2H3
InchiKey: FVJYABFEMJVLGH-UHFFFAOYSA-N
Formula: C6H10S
SMILES: CC1=C(C)CSC1
Mol. weight [g/mol]: 114.21

Physical Properties

Property code	Value	Unit	Source
gf	94.46	kJ/mol	Joback Method
hf	-6.25	kJ/mol	Joback Method
hfus	8.26	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.070		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	413.58	K	Joback Method
tc	632.63	K	Joback Method
tf	281.77	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.88	J/mol×K	413.58	Joback Method
cpg	182.34	J/mol×K	450.09	Joback Method
cpg	193.17	J/mol×K	486.60	Joback Method
cpg	203.41	J/mol×K	523.10	Joback Method
cpg	213.07	J/mol×K	559.61	Joback Method
cpg	222.19	J/mol×K	596.12	Joback Method
cpg	230.79	J/mol×K	632.63	Joback Method

Sources

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=R261375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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