2-ethyl-5-methyl-4,5-dihydrothiophen-3(2H)-one

Inchi: InChI=1S/C7H12OS/c1-3-7-6(8)4-5(2)9-7/h5,7H,3-4H2,1-2H3
InchiKey: QLSQVFFLKOOUIM-UHFFFAOYSA-N
Formula: C7H12OS
SMILES: CCC1SC(C)CC1=O
Mol. weight [g/mol]: 144.24

Physical Properties

Property code	Value	Unit	Source
gf	-45.83	kJ/mol	Joback Method
hf	-240.11	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	41.18	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.860		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1104.00		NIST Webbook
tb	485.82	K	Joback Method
tc	715.09	K	Joback Method
tf	326.98	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.05	J/mol×K	485.82	Joback Method
cpg	266.28	J/mol×K	524.03	Joback Method
cpg	280.82	J/mol×K	562.24	Joback Method
cpg	294.66	J/mol×K	600.45	Joback Method
cpg	307.79	J/mol×K	638.66	Joback Method
cpg	320.22	J/mol×K	676.87	Joback Method
cpg	331.92	J/mol×K	715.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238612&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