5-ethyldihydro-2(3H)-thiophenone

Inchi: InChI=1S/C6H10OS/c1-2-5-3-4-6(7)8-5/h5H,2-4H2,1H3
InchiKey: YPNRVDPNXSBRDG-UHFFFAOYSA-N
Formula: C6H10OS
SMILES: CCC1CCC(=O)S1
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	-46.54	kJ/mol	Joback Method
hf	-199.13	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.819		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1697.00		NIST Webbook
tb	467.61	K	Joback Method
tc	701.03	K	Joback Method
tf	319.95	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.93	J/mol×K	467.61	Joback Method
cpg	221.51	J/mol×K	506.51	Joback Method
cpg	234.44	J/mol×K	545.42	Joback Method
cpg	246.74	J/mol×K	584.32	Joback Method
cpg	258.39	J/mol×K	623.22	Joback Method
cpg	269.40	J/mol×K	662.12	Joback Method

cpg	279.76	J/mol×K	701.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301423&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume