

3(2H)-Thiophenone, 2-ethyldihydro-

Other names:	4,5-Dihydro-2-ethylthiophen-3(2H)-one Thiophen-3(2H)-one, 2-ethyl-4,5-dihydro Dihydro-2-ethyl-3(2H)-thiophenone
Inchi:	InChI=1S/C6H10OS/c1-2-6-5(7)3-4-8-6/h6H,2-4H2,1H3
InchiKey:	KNYBAJCQHFBMOP-UHFFFAOYSA-N
Formula:	C6H10OS
SMILES:	CCC1SCCC1=O
Mol. weight [g/mol]:	130.21
CAS:	52662-38-1

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	-1.50		Crippen Method
logp	1.471		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1082.00		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

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=C52662381&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

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