Dihydro-2(3H)-thiophenone

Other names:	«gamma»-Thiobutyrolactone 4-Butyrothiolactone 2(3H)-Thiophenone, dihydro- 2-Thiophenone, tetrahydro- 2-Oxothiolane Tetrahydro-2-thiophenone Thiacyclopentan-2-one Thiacyclopentanone-2 4-Thiobutyrolactone Thiolan-2-one 2-Oxotetrahydrothiophene NSC 54087
Inchi:	InChI=1S/C4H6OS/c5-4-2-1-3-6-4/h1-3H2
InchiKey:	KMSNYNIWEORQDJ-UHFFFAOYSA-N
Formula:	C4H6OS
SMILES:	O=C1CCCS1
Mol. weight [g/mol]:	102.16
CAS:	1003-10-7

Physical Properties

Property code	Value	Unit	Source
chl	-2800.00 ± 1.70	kJ/mol	NIST Webbook
gf	-55.67	kJ/mol	Joback Method
hf	-196.20 ± 2.00	kJ/mol	NIST Webbook
hfus	2.15	kJ/mol	Joback Method
hvap	38.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.040		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
rinpol	952.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1615.00		NIST Webbook
tb	426.52	K	Joback Method
tc	667.95	K	Joback Method
tf	301.65	K	Joback Method
vc	0.255	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.08	J/mol×K	426.52	Joback Method
cpg	139.26	J/mol×K	466.76	Joback Method
cpg	148.95	J/mol×K	507.00	Joback Method
cpg	158.14	J/mol×K	547.23	Joback Method
cpg	166.85	J/mol×K	587.47	Joback Method
cpg	175.06	J/mol×K	627.71	Joback Method
cpg	182.78	J/mol×K	667.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	312.70	K	0.10	NIST Webbook

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=C1003107&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume