5-hexyldihydro-2(3H)-thiophenone

Inchi: InChI=1S/C10H18OS/c1-2-3-4-5-6-9-7-8-10(11)12-9/h9H,2-8H2,1H3
InchiKey: WNKFQXYZJSZLDQ-UHFFFAOYSA-N
Formula: C10H18OS
SMILES: CCCCCCC1CCC(=O)S1
Mol. weight [g/mol]: 186.31

Physical Properties

Property code	Value	Unit	Source
gf	-12.86	kJ/mol	Joback Method
hf	-281.69	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.379		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2142.00		NIST Webbook
tb	559.13	K	Joback Method
tc	776.75	K	Joback Method
tf	365.03	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.98	J/mol×K	559.13	Joback Method
cpg	405.65	J/mol×K	595.40	Joback Method
cpg	422.41	J/mol×K	631.67	Joback Method
cpg	438.27	J/mol×K	667.94	Joback Method
cpg	453.26	J/mol×K	704.21	Joback Method
cpg	467.36	J/mol×K	740.48	Joback Method

cpg	480.62	J/mol×K	776.75	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=R301438&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume