5-octyldihydro-2(3H)-thiophenone

Inchi: InChI=1S/C12H22OS/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey: YAIREMZPYAWWGE-UHFFFAOYSA-N
Formula: C12H22OS
SMILES: CCCCCCCCC1CCC(=O)S1
Mol. weight [g/mol]: 214.37

Physical Properties

Property code	Value	Unit	Source
gf	3.98	kJ/mol	Joback Method
hf	-322.97	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	52.62	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.159		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1754.00		NIST Webbook
ripol	2382.00		NIST Webbook
tb	604.89	K	Joback Method
tc	815.27	K	Joback Method
tf	387.57	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.69	J/mol×K	604.89	Joback Method
cpg	507.56	J/mol×K	639.95	Joback Method
cpg	525.45	J/mol×K	675.02	Joback Method
cpg	542.36	J/mol×K	710.08	Joback Method
cpg	558.31	J/mol×K	745.14	Joback Method
cpg	573.33	J/mol×K	780.21	Joback Method
cpg	587.43	J/mol×K	815.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301443&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