5-Butyldihydro-2(3H)thiophenone

Inchi: InChI=1S/C8H14OS/c1-2-3-4-7-5-6-8(9)10-7/h7H,2-6H2,1H3
InchiKey: LYTJSDADPFIGCT-UHFFFAOYSA-N
Formula: C8H14OS
SMILES: CCCCC1CCC(=O)S1
Mol. weight [g/mol]: 158.26
CAS: 104223-43-0

Physical Properties

Property code	Value	Unit	Source
gf	-29.70	kJ/mol	Joback Method
hf	-240.41	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	43.72	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.599		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	513.37	K	Joback Method
tc	738.80	K	Joback Method
tf	342.49	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.10	J/mol×K	513.37	Joback Method
cpg	310.05	J/mol×K	550.94	Joback Method
cpg	325.20	J/mol×K	588.51	Joback Method
cpg	339.56	J/mol×K	626.09	Joback Method
cpg	353.14	J/mol×K	663.66	Joback Method
cpg	365.94	J/mol×K	701.23	Joback Method

cpg	377.97	J/mol×K	738.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104223430&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