5-butyl-dihydrofuran-2(3H)-thione

Inchi: InChI=1S/C8H12OS/c1-2-3-4-7-5-6-8(10)9-7/h5H,2-4,6H2,1H3
InchiKey: RGBBTFSIKXJSSL-UHFFFAOYSA-N
Formula: C8H12OS
SMILES: CCCCC1=CCC(=S)O1
Mol. weight [g/mol]: 156.25

Physical Properties

Property code	Value	Unit	Source
gf	85.80	kJ/mol	Joback Method
hf	-98.22	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.808		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1389.00		NIST Webbook
ripol	2162.00		NIST Webbook
ripol	2162.00		NIST Webbook
tb	506.12	K	Joback Method
tc	724.04	K	Joback Method
tf	298.58	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.86	J/mol×K	506.12	Joback Method
cpg	281.18	J/mol×K	542.44	Joback Method
cpg	292.71	J/mol×K	578.76	Joback Method
cpg	303.50	J/mol×K	615.08	Joback Method
cpg	313.59	J/mol×K	651.40	Joback Method
cpg	323.05	J/mol×K	687.72	Joback Method
cpg	331.93	J/mol×K	724.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422476&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