cis-5-butyl-4-methyldihydrofuran-2(3H)-thione

Inchi: InChI=1S/C9H16OS/c1-3-4-5-8-7(2)6-9(11)10-8/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey: IBXKFMLVUWMVDT-HTQZYQBOSA-N
Formula: C9H16OS
SMILES: CCCCC1OC(=S)CC1C
Mol. weight [g/mol]: 172.29

Physical Properties

Property code	Value	Unit	Source
gf	58.47	kJ/mol	Joback Method
hf	-205.85	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.929		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1430.00		NIST Webbook
ripol	2148.00		NIST Webbook
tb	515.52	K	Joback Method
tc	726.34	K	Joback Method
tf	288.09	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.76	J/mol×K	515.52	Joback Method
cpg	348.43	J/mol×K	550.66	Joback Method
cpg	363.22	J/mol×K	585.79	Joback Method
cpg	377.16	J/mol×K	620.93	Joback Method
cpg	390.30	J/mol×K	656.07	Joback Method
cpg	402.68	J/mol×K	691.21	Joback Method
cpg	414.33	J/mol×K	726.34	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R422585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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