(Z)-5-(hex-3-enyl)-5-methyl-dihydrofuran-2(3H)-thi

Inchi: InChI=1S/C11H18OS/c1-3-4-5-6-8-11(2)9-7-10(13)12-11/h4-5H,3,6-9H2,1-2H3/b5-4-
InchiKey: VCQXDKORADAQPS-PLNGDYQASA-N
Formula: C11H18OS
SMILES: CCC=CCCC1(C)CCC(=S)O1
Mol. weight [g/mol]: 198.32

Physical Properties

Property code	Value	Unit	Source
gf	157.75	kJ/mol	Joback Method
hf	-94.33	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.629		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1591.00		NIST Webbook
ripol	2335.00		NIST Webbook
tb	570.35	K	Joback Method
tc	792.47	K	Joback Method
tf	333.69	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.07	J/mol×K	570.35	Joback Method
cpg	421.96	J/mol×K	607.37	Joback Method
cpg	436.79	J/mol×K	644.39	Joback Method
cpg	450.71	J/mol×K	681.41	Joback Method
cpg	463.91	J/mol×K	718.43	Joback Method
cpg	476.56	J/mol×K	755.45	Joback Method
cpg	488.81	J/mol×K	792.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422629&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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