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

Inchi: InChI=1S/C10H16OS/c1-2-3-4-5-6-9-7-8-10(12)11-9/h7H,2-6,8H2,1H3
InchiKey: QFZICPCAFWUSMA-UHFFFAOYSA-N
Formula: C10H16OS
SMILES: CCCCCCC1=CCC(=S)O1
Mol. weight [g/mol]: 184.30

Physical Properties

Property code	Value	Unit	Source
gf	102.64	kJ/mol	Joback Method
hf	-139.50	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.588		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
ripol	2355.00		NIST Webbook
ripol	2355.00		NIST Webbook
tb	551.88	K	Joback Method
tc	762.75	K	Joback Method
tf	321.12	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.16	J/mol×K	551.88	Joback Method
cpg	372.27	J/mol×K	587.03	Joback Method
cpg	385.53	J/mol×K	622.17	Joback Method
cpg	398.00	J/mol×K	657.32	Joback Method
cpg	409.72	J/mol×K	692.46	Joback Method
cpg	420.76	J/mol×K	727.61	Joback Method

cpg	431.16	J/mol×K	762.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422505&Units=SI

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

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