6-heptyl-tetrahydropyran-2-thione

Inchi: InChI=1S/C12H22OS/c1-2-3-4-5-6-8-11-9-7-10-12(14)13-11/h11H,2-10H2,1H3
InchiKey: KFLLHCHPZXFRBY-UHFFFAOYSA-N
Formula: C12H22OS
SMILES: CCCCCCCC1CCCC(=S)O1
Mol. weight [g/mol]: 214.37

Physical Properties

Property code	Value	Unit	Source
gf	79.34	kJ/mol	Joback Method
hf	-253.59	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.243		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
ripol	2600.00		NIST Webbook
ripol	2600.00		NIST Webbook
tb	593.10	K	Joback Method
tc	801.28	K	Joback Method
tf	322.62	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.96	J/mol×K	593.10	Joback Method
cpg	496.07	J/mol×K	627.80	Joback Method
cpg	513.13	J/mol×K	662.49	Joback Method
cpg	529.21	J/mol×K	697.19	Joback Method
cpg	544.35	J/mol×K	731.89	Joback Method
cpg	558.59	J/mol×K	766.59	Joback Method
cpg	571.99	J/mol×K	801.28	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=R422530&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume