(R)-6-pentyl-5,6-dihydropyran-2-thione

Inchi: InChI=1S/C10H16OS/c1-2-3-4-6-9-7-5-8-10(12)11-9/h5,8-9H,2-4,6-7H2,1H3/t9-/m0/s1
InchiKey: CCONCZUYOJKHKW-VIFPVBQESA-N
Formula: C10H16OS
SMILES: CCCCCC1CC=CC(=S)O1
Mol. weight [g/mol]: 184.30

Physical Properties

Property code	Value	Unit	Source
gf	92.46	kJ/mol	Joback Method
hf	-154.53	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	50.56	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.239		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1578.00		NIST Webbook
ripol	2416.00		NIST Webbook
tb	546.50	K	Joback Method
tc	763.74	K	Joback Method
tf	300.84	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.19	J/mol×K	546.50	Joback Method
cpg	375.97	J/mol×K	582.71	Joback Method
cpg	390.78	J/mol×K	618.91	Joback Method
cpg	404.67	J/mol×K	655.12	Joback Method
cpg	417.70	J/mol×K	691.33	Joback Method
cpg	429.90	J/mol×K	727.54	Joback Method
cpg	441.32	J/mol×K	763.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422609&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