2-Hexyl-2H-thiapyrane

Inchi: InChI=1S/C11H18S/c1-2-3-4-5-8-11-9-6-7-10-12-11/h6-7,9-11H,2-5,8H2,1H3
InchiKey: FQVCABCCQGJOGU-UHFFFAOYSA-N
Formula: C11H18S
SMILES: CCCCCCC1C=CC=CS1
Mol. weight [g/mol]: 182.33

Physical Properties

Property code	Value	Unit	Source
gf	165.97	kJ/mol	Joback Method
hf	-55.23	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.142		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1804.00		NIST Webbook
tb	516.78	K	Joback Method
tc	727.99	K	Joback Method
tf	306.08	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.27	J/mol×K	516.78	Joback Method
cpg	384.06	J/mol×K	551.98	Joback Method
cpg	400.85	J/mol×K	587.18	Joback Method
cpg	416.66	J/mol×K	622.38	Joback Method
cpg	431.55	J/mol×K	657.58	Joback Method

cpg	445.54	J/mol×K	692.78	Joback Method
cpg	458.68	J/mol×K	727.99	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=R194671&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