2-Pentyl-2H-thiapyrane

Other names: 2-pentyl-(2H)-thiapyran
2-pentylthiapyran
Inchi: InChI=1S/C10H16S/c1-2-3-4-7-10-8-5-6-9-11-10/h5-6,8-10H,2-4,7H2,1H3
InchiKey: WIWJPSVDDXGSQF-UHFFFAOYSA-N
Formula: C10H16S
SMILES: CCCCCC1C=CC=CS1
Mol. weight [g/mol]: 168.30

Physical Properties

Property code	Value	Unit	Source
gf	157.55	kJ/mol	Joback Method
hf	-34.59	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.752		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1337.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	493.90	K	Joback Method
tc	708.45	K	Joback Method
tf	294.81	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.98	J/mol×K	493.90	Joback Method
cpg	336.99	J/mol×K	529.66	Joback Method

cpg	353.02	J/mol×K	565.42	Joback Method
cpg	368.12	J/mol×K	601.17	Joback Method
cpg	382.32	J/mol×K	636.93	Joback Method
cpg	395.66	J/mol×K	672.69	Joback Method
cpg	408.17	J/mol×K	708.45	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=R180479&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

Latest version available from:
https://www.chemeo.com/cid/66-167-4/2-Pentyl-2H-thiapyrane.pdf
Generated by Cheméo on 2024-04-27 07:27:43.985645689 +0000 UTC m=+16492112.906223001.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.