

2-Butyl-2H-thiapyrane

Other names:	2-butyl-(2H)-thiapyran
Inchi:	InChI=1S/C9H14S/c1-2-3-6-9-7-4-5-8-10-9/h4-5,7-9H,2-3,6H2,1H3
InchiKey:	GLNHYDJALZRGEH-UHFFFAOYSA-N
Formula:	C9H14S
SMILES:	CCCCC1C=CC=CS1
Mol. weight [g/mol]:	154.27

Physical Properties

Property code	Value	Unit	Source
gf	149.13	kJ/mol	Joback Method
hf	-13.95	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.362		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1223.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1597.00		NIST Webbook
tb	471.02	K	Joback Method
tc	688.90	K	Joback Method
tf	283.54	K	Joback Method
vc	0.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.55	J/molxK	471.02	Joback Method
cpg	291.64	J/molxK	507.33	Joback Method

cpg	306.80	J/mol×K	543.65	Joback Method
cpg	321.06	J/mol×K	579.96	Joback Method
cpg	334.46	J/mol×K	616.27	Joback Method
cpg	347.04	J/mol×K	652.59	Joback Method
cpg	358.82	J/mol×K	688.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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