

Thiophene, 2-butyltetrahydro-

Other names:	2-Butyltetrahydrothiophene 2-Butylthiacyclopentane 2-Butylthiophane 2-Butyl-thiolane Thiolane, 2-butyl
Inchi:	InChI=1S/C8H16S/c1-2-3-5-8-6-4-7-9-8/h8H,2-7H2,1H3
InchiKey:	NBPQJOLVXAKDFK-UHFFFAOYSA-N
Formula:	C8H16S
SMILES:	CCCCC1CCCS1
Mol. weight [g/mol]:	144.28
CAS:	1613-49-6

Physical Properties

Property code	Value	Unit	Source
gf	92.89	kJ/mol	Joback Method
hf	-102.71	kJ/mol	Joback Method
hfus	14.07	kJ/mol	Joback Method
hvap	39.47	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.072		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook

rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
tb	445.55	K	Joback Method
tc	653.61	K	Joback Method
tf	274.27	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.40	J/mol×K	445.55	Joback Method
cpg	280.01	J/mol×K	480.23	Joback Method
cpg	295.73	J/mol×K	514.90	Joback Method
cpg	310.61	J/mol×K	549.58	Joback Method
cpg	324.67	J/mol×K	584.26	Joback Method
cpg	337.94	J/mol×K	618.93	Joback Method
cpg	350.47	J/mol×K	653.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613496&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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