Butylthiobenzene

Other names:	Benzene, (butylthio)-
	Sulfide, butyl phenyl
	Butyl phenyl sulfide
	Phenyl butyl sulfide
	(n-Butylthio)benzene
	(1-Thiapentyl)benzene
	n-Butyl phenyl sulfide
	Benzenethiol, S-n-butyl-
Inchi:	InChI=1S/C10H14S/c1-2-3-9-11-10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3
InchiKey:	JETFNRIIPBNRAT-UHFFFAOYSA-N
Formula:	C10H14S
SMILES:	CCCCSc1ccccc1
Mol. weight [g/mol]:	166.28
CAS:	1126-80-3

Physical Properties

Property code	Value	Unit	Source
gf	178.85	kJ/mol	Joback Method
hf	28.67	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	46.95	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.579		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	523.66	K	Joback Method
tc	750.09	K	Joback Method
tf	263.28	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.71	J/mol×K	523.66	Joback Method
cpg	325.11	J/mol×K	561.40	Joback Method
cpg	339.56	J/mol×K	599.14	Joback Method
cpg	353.09	J/mol×K	636.88	Joback Method
cpg	365.75	J/mol×K	674.62	Joback Method
cpg	377.55	J/mol×K	712.35	Joback Method
cpg	388.54	J/mol×K	750.09	Joback Method

Sources

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=C1126803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.