Benzene, [(1-methylpropyl)thio]-

Other names:	Sulfide, sec-butyl phenyl
	sec-Butyl phenyl sulfide
	Phenyl sec-butyl sulfide
	2-(Phenylthio)butane
	(sec-Butylthio)benzene
	(2-Methyl-1-thiabutyl)benzene
	2-Methyl-1-(1-thiabutyl)benzene
Inchi:	InChI=1S/C10H14S/c1-3-9(2)11-10-7-5-4-6-8-10/h4-9H,3H2,1-2H3
InchiKey:	YKLUJQMOFAXHHI-UHFFFAOYSA-N
Formula:	C10H14S
SMILES:	CCC(C)Sc1ccccc1
Mol. weight [g/mol]:	166.28
CAS:	14905-79-4

Physical Properties

Property code	Value	Unit	Source
gf	176.41	kJ/mol	Joback Method
hf	23.39	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.577		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
tb	523.22	K	Joback Method
tc	754.96	K	Joback Method
tf	248.28	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	310.00	J/mol×K	523.22	Joback Method
cpg	325.83	J/mol×K	561.84	Joback Method
cpg	340.66	J/mol×K	600.47	Joback Method
cpg	354.52	J/mol×K	639.09	Joback Method
cpg	367.45	J/mol×K	677.71	Joback Method
cpg	379.48	J/mol×K	716.34	Joback Method
cpg	390.65	J/mol×K	754.96	Joback Method

Sources

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=C14905794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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