Benzene, [(2-methylpropyl)thio]-

Other names:	Sulfide, isobutyl phenyl
	Isobutyl phenyl sulfide
	isobutylthiobenzene
Inchi:	InChI=1S/C10H14S/c1-9(2)8-11-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	UQRLAGGSKUVKMJ-UHFFFAOYSA-N
Formula:	C10H14S
SMILES:	CC(C)CSc1ccccc1
Mol. weight [g/mol]:	166.28
CAS:	13307-61-4

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	-3.23		Crippen Method
logp	3.435		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1303.00		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:	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=C13307614&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume