Benzene, [(1,1-dimethylethyl)thio]-

Other names: Sulfide, tert-butyl phenyl
tert-Butyl Phenyl sulfide
Phenyl tert-butyl sulfide
Inchi: InChI=1S/C10H14S/c1-10(2,3)11-9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey: VEUCZKAZCRSEMP-UHFFFAOYSA-N
Formula: C10H14S
SMILES: CC(C)(C)Sc1ccccc1
Mol. weight [g/mol]: 166.28
CAS: 3019-19-0

Physical Properties

Property code	Value	Unit	Source
gf	181.69	kJ/mol	Joback Method
hf	19.92	kJ/mol	Joback Method
hfus	12.41	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
ie	8.20 ± 0.10	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.38 ± 0.05	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	3.577		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
tb	520.43	K	Joback Method
tc	762.39	K	Joback Method
tf	265.70	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.97	J/mol×K	520.43	Joback Method

cpg	329.60	J/mol×K	560.76	Joback Method
cpg	344.99	J/mol×K	601.08	Joback Method
cpg	359.19	J/mol×K	641.41	Joback Method
cpg	372.29	J/mol×K	681.74	Joback Method
cpg	384.34	J/mol×K	722.06	Joback Method
cpg	395.43	J/mol×K	762.39	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=C3019190&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
ie:	Ionization energy
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