Benzene, 1-methyl-3-[(1-methylethyl)thio]-

Other names: Sulfide, isopropyl m-tolyl
Isopropyl m-tolyl sulfide
Inchi: InChI=1S/C10H14S/c1-8(2)11-10-6-4-5-9(3)7-10/h4-8H,1-3H3
InchiKey: CIUOVJDIRUPGIE-UHFFFAOYSA-N
Formula: C10H14S
SMILES: Cc1cccc(SC(C)C)c1
Mol. weight [g/mol]: 166.28
CAS: 14905-80-7

Physical Properties

Property code	Value	Unit	Source
gf	166.78	kJ/mol	Joback Method
hf	11.92	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
ie	8.38	eV	NIST Webbook
log10ws	-3.64		Crippen Method
logp	3.496		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	528.20	K	Joback Method
tc	761.14	K	Joback Method
tf	260.80	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.01	J/mol×K	528.20	Joback Method
cpg	325.47	J/mol×K	567.02	Joback Method
cpg	339.98	J/mol×K	605.85	Joback Method
cpg	353.59	J/mol×K	644.67	Joback Method
cpg	366.32	J/mol×K	683.50	Joback Method
cpg	378.20	J/mol×K	722.32	Joback Method

cpg	389.25	J/mol×K	761.14	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=C14905807&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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