Benzene, [2-[(1-methylethyl)thio]ethyl]-

Other names: 2-(1-Methylethylthio)ethylbenzene
Inchi: InChI=1S/C11H16S/c1-10(2)12-9-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey: MJLYFFRRKQGUDV-UHFFFAOYSA-N
Formula: C11H16S
SMILES: CC(C)SCCc1ccccc1
Mol. weight [g/mol]: 180.31
CAS: 54576-42-0

Physical Properties

Property code	Value	Unit	Source
gf	184.83	kJ/mol	Joback Method
hf	2.75	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
ie	8.26	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-3.53		Crippen Method
logp	3.371		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	546.10	K	Joback Method
tc	773.53	K	Joback Method
tf	259.55	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.19	J/mol×K	546.10	Joback Method
cpg	372.85	J/mol×K	584.01	Joback Method
cpg	388.47	J/mol×K	621.91	Joback Method
cpg	403.08	J/mol×K	659.82	Joback Method
cpg	416.73	J/mol×K	697.72	Joback Method
cpg	429.44	J/mol×K	735.63	Joback Method

cpg	441.26	J/mol×K	773.53	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=C54576420&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