Benzene, 1,2-bis-(methylthio)ethyl

Inchi: InChI=1S/C10H14S2/c1-11-8-10(12-2)9-6-4-3-5-7-9/h3-7,10H,8H2,1-2H3
InchiKey: ILDMWBMAZPQGPE-UHFFFAOYSA-N
Formula: C10H14S2
SMILES: CSCC(SC)c1ccccc1
Mol. weight [g/mol]: 198.35

Physical Properties

Property code	Value	Unit	Source
gf	209.53	kJ/mol	Joback Method
hf	65.26	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	53.38	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.454		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	592.00	K	Joback Method
tc	844.18	K	Joback Method
tf	282.68	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.14	J/mol×K	592.00	Joback Method
cpg	377.93	J/mol×K	634.03	Joback Method
cpg	392.57	J/mol×K	676.06	Joback Method
cpg	406.09	J/mol×K	718.09	Joback Method
cpg	418.52	J/mol×K	760.12	Joback Method
cpg	429.91	J/mol×K	802.15	Joback Method
cpg	440.28	J/mol×K	844.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121663&Units=SI
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

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