Benzene, 1-methoxy-4-[1,2-bis-(methylthio)propyl], erythro

Inchi: InChI=1S/C12H18OS2/c1-9(14-3)12(15-4)10-5-7-11(13-2)8-6-10/h5-9,12H,1-4H3/t9-,12-

InchiKey: XDYCLYJKOXFBFP-CABZTGNLSA-N

Formula: C12H18OS2

SMILES: COc1ccc(C(SC)C(C)SC)cc1

Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	109.30	kJ/mol	Joback Method
hf	-124.99	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.851		Crippen Method
mcvol	194.750	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1919.00		NIST Webbook
tb	664.72	K	Joback Method
tc	908.15	K	Joback Method
tf	324.97	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.33	J/mol×K	664.72	Joback Method
cpg	503.11	J/mol×K	705.29	Joback Method
cpg	518.69	J/mol×K	745.86	Joback Method
cpg	533.08	J/mol×K	786.43	Joback Method
cpg	546.30	J/mol×K	827.01	Joback Method
cpg	558.34	J/mol×K	867.58	Joback Method
cpg	569.22	J/mol×K	908.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121678&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

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