Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-4-(methylthio)

Inchi: InChI=1S/C13H18S/c1-10(13(2,3)4)11-6-8-12(14-5)9-7-11/h6-9H,1H2,2-5H3
InchiKey: RYYOLWGCONEHGL-UHFFFAOYSA-N
Formula: C13H18S
SMILES: C=C(c1ccc(SC)cc1)C(C)(C)C
Mol. weight [g/mol]: 206.35
CAS: 146558-39-6

Physical Properties

Property code	Value	Unit	Source
affp	894.80	kJ/mol	NIST Webbook
basg	866.00	kJ/mol	NIST Webbook
gf	276.61	kJ/mol	Joback Method
hf	62.17	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	52.40	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.468		Crippen Method
mcvol	182.320	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	590.61	K	Joback Method
tc	829.03	K	Joback Method
tf	296.31	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.17	J/mol×K	590.61	Joback Method
cpg	453.08	J/mol×K	630.35	Joback Method
cpg	469.69	J/mol×K	670.08	Joback Method
cpg	485.07	J/mol×K	709.82	Joback Method
cpg	499.31	J/mol×K	749.56	Joback Method
cpg	512.49	J/mol×K	789.29	Joback Method
cpg	524.68	J/mol×K	829.03	Joback Method

Sources

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=C146558396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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