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

Other names: Benzene, 1-[(1,1-dimethylethyl)thio]-3-methyl-
Inchi: InChI=1S/C11H16S/c1-9-6-5-7-10(8-9)12-11(2,3)4/h5-8H,1-4H3
InchiKey: NOSDQZYLLGTSNW-UHFFFAOYSA-N
Formula: C11H16S
SMILES: Cc1cccc(SC(C)(C)C)c1
Mol. weight [g/mol]: 180.32

Physical Properties

Property code	Value	Unit	Source
af	0.3364		Cheméo Relay (1.0)
gf	180.48	kJ/mol	Joback Method
hf	-29.81	kJ/mol	Cheméo Relay (1.0)
hfus	14.61	kJ/mol	Joback Method
hvap	56.79	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	NIST Webbook
log10ws	-4.37		Cheméo Relay (1.0)
logp	3.886		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	511.43	K	Cheméo Relay (1.0)
tc	703.82	K	Cheméo Relay (1.0)
tf	279.68	K	Cheméo Relay (1.0)
vc	0.573	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.12	J/mol×K	548.29	Joback Method
cpg	376.14	J/mol×K	588.01	Joback Method
cpg	391.96	J/mol×K	627.73	Joback Method
cpg	406.64	J/mol×K	667.45	Joback Method
cpg	420.24	J/mol×K	707.18	Joback Method
cpg	432.83	J/mol×K	746.90	Joback Method
cpg	444.47	J/mol×K	786.62	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34786260&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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