Benzoic acid, 4-(methylthio)-, 1-methylpropyl ester

Inchi: InChI=1S/C12H16O2S/c1-4-9(2)14-12(13)10-5-7-11(15-3)8-6-10/h5-9H,4H2,1-3H3
InchiKey: XMQNLDGBHVGQHD-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CCC(C)OC(=O)c1ccc(SC)cc1
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-50.30	kJ/mol	Joback Method
hf	-274.16	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.364		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1785.00		NIST Webbook
tb	650.25	K	Joback Method
tc	878.49	K	Joback Method
tf	355.50	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.59	J/mol×K	650.25	Joback Method
cpg	463.72	J/mol×K	688.29	Joback Method
cpg	477.86	J/mol×K	726.33	Joback Method
cpg	491.02	J/mol×K	764.37	Joback Method
cpg	503.21	J/mol×K	802.41	Joback Method
cpg	514.45	J/mol×K	840.45	Joback Method
cpg	524.75	J/mol×K	878.49	Joback Method

Sources

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=U375361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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