Benzoic acid, 4-(isopropylthio)-, isopropyl ester

Inchi: InChI=1S/C13H18O2S/c1-9(2)15-13(14)11-5-7-12(8-6-11)16-10(3)4/h5-10H,1-4H3
InchiKey: CVSBRDUPDMNVGA-UHFFFAOYSA-N
Formula: C13H18O2S
SMILES: CC(C)OC(=O)c1ccc(SC(C)C)cc1
Mol. weight [g/mol]: 238.35

Physical Properties

Property code	Value	Unit	Source
gf	-44.32	kJ/mol	Joback Method
hf	-300.08	kJ/mol	Joback Method
hfus	22.95	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.752		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1757.00		NIST Webbook
tb	672.69	K	Joback Method
tc	901.16	K	Joback Method
tf	351.77	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.34	J/mol×K	672.69	Joback Method
cpg	516.33	J/mol×K	710.77	Joback Method
cpg	531.24	J/mol×K	748.85	Joback Method
cpg	545.08	J/mol×K	786.92	Joback Method
cpg	557.87	J/mol×K	825.00	Joback Method
cpg	569.62	J/mol×K	863.08	Joback Method
cpg	580.37	J/mol×K	901.16	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=U375406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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