Benzoic acid, 2-(isopropylthio)-

Inchi: InChI=1S/C10H12O2S/c1-7(2)12-10(11)8-5-3-4-6-9(8)13/h3-7,13H,1-2H3
InchiKey: KIFAIZBEBNZNBY-UHFFFAOYSA-N
Formula: C10H12O2S
SMILES: CC(C)OC(=O)c1ccccc1S
Mol. weight [g/mol]: 196.27

Physical Properties

Property code	Value	Unit	Source
gf	-70.87	kJ/mol	Joback Method
hf	-236.27	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	56.30	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.541		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	598.57	K	Joback Method
tc	836.81	K	Joback Method
tf	335.02	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.05	J/mol×K	598.57	Joback Method
cpg	361.71	J/mol×K	638.28	Joback Method
cpg	374.48	J/mol×K	677.98	Joback Method
cpg	386.36	J/mol×K	717.69	Joback Method
cpg	397.38	J/mol×K	757.40	Joback Method
cpg	407.56	J/mol×K	797.10	Joback Method
cpg	416.92	J/mol×K	836.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375412&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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