Benzoic acid, 2-(methylthio)-, tert.-butyl ester

Inchi: InChI=1S/C12H16O2S/c1-12(2,3)14-11(13)9-7-5-6-8-10(9)15-4/h5-8H,1-4H3
InchiKey: VYARXAMJCOZNEA-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CSc1ccccc1C(=O)OC(C)(C)C
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-45.02	kJ/mol	Joback Method
hf	-277.63	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.364		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	647.46	K	Joback Method
tc	884.57	K	Joback Method
tf	372.92	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.26	J/mol×K	647.46	Joback Method
cpg	466.71	J/mol×K	686.98	Joback Method
cpg	481.03	J/mol×K	726.50	Joback Method
cpg	494.25	J/mol×K	766.01	Joback Method
cpg	506.42	J/mol×K	805.53	Joback Method
cpg	517.59	J/mol×K	845.05	Joback Method
cpg	527.78	J/mol×K	884.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375371&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