Benzoic acid, 2-(methylthio)-, methyl ester

Inchi: InChI=1S/C9H10O2S/c1-11-9(10)7-5-3-4-6-8(7)12-2/h3-6H,1-2H3
InchiKey: CPQDZXPLQXZJGF-UHFFFAOYSA-N
Formula: C9H10O2S
SMILES: COC(=O)c1ccccc1SC
Mol. weight [g/mol]: 182.24
CAS: 3704-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-73.12	kJ/mol	Joback Method
hf	-206.96	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.195		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1554.60		NIST Webbook
tb	582.05	K	Joback Method
tc	819.33	K	Joback Method
tf	336.69	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.44	J/mol×K	582.05	Joback Method
cpg	315.94	J/mol×K	621.60	Joback Method
cpg	327.66	J/mol×K	661.14	Joback Method
cpg	338.59	J/mol×K	700.69	Joback Method
cpg	348.75	J/mol×K	740.23	Joback Method
cpg	358.12	J/mol×K	779.78	Joback Method
cpg	366.72	J/mol×K	819.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3704287&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