Benzoic acid, 3-(methylthio)-, isopropyl ester

Inchi: InChI=1S/C11H14O2S/c1-8(2)13-11(12)9-5-4-6-10(7-9)14-3/h4-8H,1-3H3
InchiKey: HVJICQIHGZIGTI-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: CSc1cccc(C(=O)OC(C)C)c1
Mol. weight [g/mol]: 210.29

Physical Properties

Property code	Value	Unit	Source
gf	-58.72	kJ/mol	Joback Method
hf	-253.52	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.974		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	627.37	K	Joback Method
tc	860.16	K	Joback Method
tf	344.23	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.78	J/mol×K	627.37	Joback Method
cpg	413.29	J/mol×K	666.17	Joback Method
cpg	426.85	J/mol×K	704.97	Joback Method
cpg	439.46	J/mol×K	743.76	Joback Method
cpg	451.15	J/mol×K	782.56	Joback Method
cpg	461.92	J/mol×K	821.36	Joback Method
cpg	471.77	J/mol×K	860.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375368&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

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