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

Inchi: InChI=1S/C10H12O2S/c1-3-12-10(11)8-5-4-6-9(7-8)13-2/h4-7H,3H2,1-2H3
InchiKey: DXATWXQPWLCGPA-UHFFFAOYSA-N
Formula: C10H12O2S
SMILES: CCOC(=O)c1cccc(SC)c1
Mol. weight [g/mol]: 196.27

Physical Properties

Property code	Value	Unit	Source
gf	-64.70	kJ/mol	Joback Method
hf	-227.60	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.585		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	604.93	K	Joback Method
tc	837.42	K	Joback Method
tf	347.96	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.05	J/mol×K	604.93	Joback Method
cpg	363.45	J/mol×K	643.68	Joback Method
cpg	376.01	J/mol×K	682.43	Joback Method
cpg	387.72	J/mol×K	721.18	Joback Method
cpg	398.60	J/mol×K	759.92	Joback Method
cpg	408.65	J/mol×K	798.67	Joback Method
cpg	417.88	J/mol×K	837.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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