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

Inchi: InChI=1S/C11H14O2S/c1-3-7-13-11(12)9-5-4-6-10(8-9)14-2/h4-6,8H,3,7H2,1-2H3
InchiKey: QICWHAVUFFJEEW-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: CCCOC(=O)c1cccc(SC)c1
Mol. weight [g/mol]: 210.29

Physical Properties

Property code	Value	Unit	Source
gf	-56.28	kJ/mol	Joback Method
hf	-248.24	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.975		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	627.81	K	Joback Method
tc	855.76	K	Joback Method
tf	359.23	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.30	J/mol×K	627.81	Joback Method
cpg	412.46	J/mol×K	665.80	Joback Method
cpg	425.72	J/mol×K	703.79	Joback Method
cpg	438.10	J/mol×K	741.78	Joback Method
cpg	449.59	J/mol×K	779.77	Joback Method
cpg	460.21	J/mol×K	817.77	Joback Method
cpg	469.97	J/mol×K	855.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374953&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