Benzoic acid, 4-(methylthio)-, butyl ester

Inchi: InChI=1S/C12H16O2S/c1-3-4-9-14-12(13)10-5-7-11(15-2)8-6-10/h5-8H,3-4,9H2,1-2H3
InchiKey: DNKZZKUGJNNTDO-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CCCCOC(=O)c1ccc(SC)cc1
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-47.86	kJ/mol	Joback Method
hf	-268.88	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.365		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	650.69	K	Joback Method
tc	874.38	K	Joback Method
tf	370.50	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.09	J/mol×K	650.69	Joback Method
cpg	462.89	J/mol×K	687.97	Joback Method
cpg	476.74	J/mol×K	725.25	Joback Method
cpg	489.66	J/mol×K	762.53	Joback Method
cpg	501.66	J/mol×K	799.81	Joback Method
cpg	512.76	J/mol×K	837.10	Joback Method
cpg	522.97	J/mol×K	874.38	Joback Method

Sources

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=U374945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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