Benzoic acid, 3-(methylthio)-, 2-methylbutyl ester

Inchi: InChI=1S/C13H18O2S/c1-4-10(2)9-15-13(14)11-6-5-7-12(8-11)16-3/h5-8,10H,4,9H2,1-3

InchiKey: XTFZZZVYNKLXEJ-UHFFFAOYSA-N

Formula: C13H18O2S

SMILES: CCC(C)COC(=O)c1cccc(SC)c1

Mol. weight [g/mol]: 238.35

Physical Properties

Property code	Value	Unit	Source
gf	-41.88	kJ/mol	Joback Method
hf	-294.80	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.611		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1876.00		NIST Webbook
tb	673.13	K	Joback Method
tc	897.16	K	Joback Method
tf	366.77	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.83	J/mol×K	673.13	Joback Method
cpg	515.48	J/mol×K	710.47	Joback Method
cpg	530.10	J/mol×K	747.81	Joback Method
cpg	543.70	J/mol×K	785.14	Joback Method
cpg	556.31	J/mol×K	822.48	Joback Method
cpg	567.93	J/mol×K	859.82	Joback Method
cpg	578.59	J/mol×K	897.16	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=U375366&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