Benzoic acid, 2-(2-methylpropyl)thio-, 2-methylpropyl ester

Inchi: InChI=1S/C15H22O2S/c1-11(2)9-17-15(16)13-7-5-6-8-14(13)18-10-12(3)4/h5-8,11-12H,9

InchiKey: DGVNKUKXMRWPMP-UHFFFAOYSA-N

Formula: C15H22O2S

SMILES: CC(C)COC(=O)c1ccccc1SCC(C)C

Mol. weight [g/mol]: 266.40

Physical Properties

Property code	Value	Unit	Source
gf	-27.48	kJ/mol	Joback Method
hf	-341.36	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	67.12	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.247		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	718.45	K	Joback Method
tc	939.03	K	Joback Method
tf	374.31	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.78	J/mol×K	718.45	Joback Method
cpg	623.50	J/mol×K	755.21	Joback Method
cpg	639.07	J/mol×K	791.98	Joback Method
cpg	653.53	J/mol×K	828.74	Joback Method
cpg	666.90	J/mol×K	865.51	Joback Method
cpg	679.19	J/mol×K	902.27	Joback Method
cpg	690.43	J/mol×K	939.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375414&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