Benzoic acid, 3-(3-methylbutyl)thio-, 3-methylbutyl ester

Inchi: InChI=1S/C17H26O2S/c1-13(2)8-10-19-17(18)15-6-5-7-16(12-15)20-11-9-14(3)4/h5-7,12

InchiKey: NLIZJRLTRIFMEW-UHFFFAOYSA-N

Formula: C17H26O2S

SMILES: CC(C)CCOC(=O)c1cccc(SCCC(C)C)c1

Mol. weight [g/mol]: 294.45

Physical Properties

Property code	Value	Unit	Source
gf	-10.64	kJ/mol	Joback Method
hf	-382.64	kJ/mol	Joback Method
hfus	33.31	kJ/mol	Joback Method
hvap	71.57	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.028		Crippen Method
mcvol	250.420	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
tb	764.21	K	Joback Method
tc	978.68	K	Joback Method
tf	396.85	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.88	J/mol×K	764.21	Joback Method
cpg	735.04	J/mol×K	799.95	Joback Method
cpg	751.02	J/mol×K	835.70	Joback Method
cpg	765.84	J/mol×K	871.44	Joback Method
cpg	779.53	J/mol×K	907.19	Joback Method
cpg	792.12	J/mol×K	942.93	Joback Method
cpg	803.63	J/mol×K	978.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375399&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