Benzoic acid, 2-(2-methylbutyl)thio-

Inchi: InChI=1S/C12H16O2S/c1-3-9(2)8-14-12(13)10-6-4-5-7-11(10)15/h4-7,9,15H,3,8H2,1-2H
InchiKey: MCCQSPCDUGUPLU-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CCC(C)COC(=O)c1ccccc1S
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-54.03	kJ/mol	Joback Method
hf	-277.55	kJ/mol	Joback Method
hfus	23.79	kJ/mol	Joback Method
hvap	60.75	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.178		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1907.00		NIST Webbook
tb	644.33	K	Joback Method
tc	873.13	K	Joback Method
tf	357.56	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.52	J/mol×K	644.33	Joback Method
cpg	460.60	J/mol×K	682.46	Joback Method
cpg	474.70	J/mol×K	720.60	Joback Method
cpg	487.84	J/mol×K	758.73	Joback Method
cpg	500.04	J/mol×K	796.86	Joback Method
cpg	511.33	J/mol×K	834.99	Joback Method
cpg	521.74	J/mol×K	873.13	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=U375409&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