

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

Inchi:	InChI=1S/C17H26O2S/c1-5-13(3)11-19-17(18)15-8-7-9-16(10-15)20-12-14(4)6-2/h7-10,1
InchiKey:	XQMMKXOIOWQZIN-UHFFFAOYSA-N
Formula:	C17H26O2S
SMILES:	CCC(C)COC(=O)c1cccc(SCC(C)CC)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
rinpola	2166.00		NIST Webbook
rinpola	2166.00		NIST Webbook
tb	764.21	K	Joback Method
tc	978.68	K	Joback Method
tf	396.85	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.88	J/molxK	764.21	Joback Method
cpg	735.04	J/molxK	799.95	Joback Method
cpg	751.02	J/molxK	835.70	Joback Method
cpg	765.84	J/molxK	871.44	Joback Method
cpg	779.53	J/molxK	907.19	Joback Method
cpg	792.12	J/molxK	942.93	Joback Method
cpg	803.63	J/molxK	978.68	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=U375382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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