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

Inchi: InChI=1S/C17H27NO2/c1-13(2)8-10-18-16-7-5-6-15(12-16)17(19)20-11-9-14(3)4/h5-7,12

InchiKey: WUTNBMJQISKMNE-UHFFFAOYSA-N

Formula: C17H27NO2

SMILES: CC(C)CCNc1cccc(C(=O)OCCC(C)C)c1

Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	45.63	kJ/mol	Joback Method
hf	-371.04	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.348		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2193.00		NIST Webbook
tb	745.60	K	Joback Method
tc	947.13	K	Joback Method
tf	415.11	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.08	J/mol×K	745.60	Joback Method
cpg	732.26	J/mol×K	779.19	Joback Method
cpg	748.38	J/mol×K	812.78	Joback Method
cpg	763.48	J/mol×K	846.36	Joback Method
cpg	777.58	J/mol×K	879.95	Joback Method
cpg	790.71	J/mol×K	913.54	Joback Method
cpg	802.91	J/mol×K	947.13	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=U375448&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