Benzoic acid, 3-(2-methylpropyl)amino-, 2-methylpropyl ester

Inchi: InChI=1S/C15H23NO2/c1-11(2)9-16-14-7-5-6-13(8-14)15(17)18-10-12(3)4/h5-8,11-12,16

InchiKey: DSEMMODTCBEYPS-UHFFFAOYSA-N

Formula: C15H23NO2

SMILES: CC(C)CNc1cccc(C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 249.35

Physical Properties

Property code	Value	Unit	Source
gf	28.79	kJ/mol	Joback Method
hf	-329.76	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	66.74	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.567		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1965.00		NIST Webbook
tb	699.84	K	Joback Method
tc	905.60	K	Joback Method
tf	392.57	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.89	J/mol×K	699.84	Joback Method
cpg	620.52	J/mol×K	734.13	Joback Method
cpg	636.13	J/mol×K	768.43	Joback Method
cpg	650.76	J/mol×K	802.72	Joback Method
cpg	664.43	J/mol×K	837.01	Joback Method
cpg	677.17	J/mol×K	871.31	Joback Method
cpg	689.00	J/mol×K	905.60	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375457&Units=SI

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