

Benzoic acid, 4-(1-methylpropyl)amino-, 1-methylpropyl ester

Inchi:	InChI=1S/C15H23NO2/c1-5-11(3)16-14-9-7-13(8-10-14)15(17)18-12(4)6-2/h7-12,16H,5-
InchiKey:	UKJMFUKMDILPQR-UHFFFAOYSA-N
Formula:	C15H23NO2
SMILES:	CCC(C)Nc1ccc(C(=O)OC(C)CC)cc1
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	-4.46		Crippen Method
logp	3.852		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		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/molxK	699.84	Joback Method
cpg	620.52	J/molxK	734.13	Joback Method
cpg	636.13	J/molxK	768.43	Joback Method
cpg	650.76	J/molxK	802.72	Joback Method
cpg	664.43	J/molxK	837.01	Joback Method
cpg	677.17	J/molxK	871.31	Joback Method
cpg	689.00	J/molxK	905.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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