Benzoic acid, 2-(1-methylpropyl)amino-

Inchi: InChI=1S/C11H15NO2/c1-3-8(2)12-10-7-5-4-6-9(10)11(13)14/h4-8,12H,3H2,1-2H3,(H,13
InchiKey: SQURSWNVGJILTD-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCC(C)Nc1ccccc1C(=O)O
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
gf	-34.27	kJ/mol	Joback Method
hf	-261.93	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.595		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	678.52	K	Joback Method
tc	881.02	K	Joback Method
tf	401.08	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.24	J/mol×K	678.52	Joback Method
cpg	436.09	J/mol×K	712.27	Joback Method
cpg	447.20	J/mol×K	746.02	Joback Method
cpg	457.61	J/mol×K	779.77	Joback Method
cpg	467.35	J/mol×K	813.52	Joback Method
cpg	476.45	J/mol×K	847.27	Joback Method
cpg	484.93	J/mol×K	881.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375348&Units=SI
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

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