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

Inchi: InChI=1S/C12H17NO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7,13H2,1-2
InchiKey: VYLQTAQLGFRYBN-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CC(C)CCOC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	-16.97	kJ/mol	Joback Method
hf	-282.24	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.472		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	654.00	K	Joback Method
tc	872.68	K	Joback Method
tf	404.36	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.19	J/mol×K	654.00	Joback Method
cpg	470.89	J/mol×K	690.45	Joback Method
cpg	484.67	J/mol×K	726.89	Joback Method
cpg	497.54	J/mol×K	763.34	Joback Method
cpg	509.54	J/mol×K	799.79	Joback Method
cpg	520.69	J/mol×K	836.23	Joback Method
cpg	531.01	J/mol×K	872.68	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=U375450&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