Isobutamben

Other names:	Benzoic acid, 4-amino-, 2-methylpropyl ester
	Benzoic acid, p-amino-, isobutyl ester
	Benzamelid
	Cicloforme
	Cyclocaine
	Cycloform
	Cyclogesin
	Isobutyl p-aminobenzoate
	Isobutyl Keloform
	Isobutyl 4-aminobenzoate
	Isobutylcaine
	Isocaine
	p-Aminobenzoic acid isobutyl ester
	Benzoic acid, p-amino-, 2-methylpropyl ester
	(2-Methylpropyl) p-aminobenzoate
	Isobutambene
	Isobutyl p-aminobenzobenzoate
	NSC 23517
	4-Aminobenzoic acid, 2-methylpropyl ester
Inchi:	InChI=1S/C11H15NO2/c1-8(2)7-14-11(13)9-3-5-10(12)6-4-9/h3-6,8H,7,12H2,1-2H3
InchiKey:	PUYOAVGNCWPANW-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CC(C)COC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	193.24
CAS:	94-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-25.39	kJ/mol	Joback Method
hf	-261.60	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.082		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1795.00		NIST Webbook

rinpol	1795.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	631.12	K	Joback Method
tc	853.74	K	Joback Method
tf	393.09	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.93	J/mol×K	816.63	Joback Method
cpg	406.12	J/mol×K	631.12	Joback Method
cpg	420.21	J/mol×K	668.22	Joback Method
cpg	433.41	J/mol×K	705.33	Joback Method
cpg	445.76	J/mol×K	742.43	Joback Method
cpg	457.25	J/mol×K	779.53	Joback Method
cpg	477.80	J/mol×K	853.74	Joback Method
hfust	10.70	kJ/mol	327.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94144&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
hfust: Enthalpy of fusion at a given temperature

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