

Benzoic acid, 2-amino-, 2-methylpropyl ester

Other names:	Anthranilic acid, isobutyl ester Isobutyl anthranilate Isobutyl o-aminobenzoate Anthranilic acid, 2-methylpropyl ester Isobutyl 2-aminobenzoate
Inchi:	InChI=1S/C11H15NO2/c1-8(2)7-14-11(13)9-5-3-4-6-10(9)12/h3-6,8H,7,12H2,1-2H3
InchiKey:	ILCLJQFCMRCPNM-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CC(C)COC(=O)c1ccccc1N
Mol. weight [g/mol]:	193.24
CAS:	7779-77-3

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	1598.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2347.00		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	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	467.93	J/mol×K	816.63	Joback Method
cpg	477.80	J/mol×K	853.74	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=C7779773&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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