benzocaine

Other names:	4-aminobenzoic acid, ethyl ester
	Benzoic acid, 4-amino-, ethyl ester
	Ethyl-p-aminobenzoate
	ethyl 4-aminobenzoate
	ethyl p-aminobenzoate
Inchi:	InChI=1S/C9H11NO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3
InchiKey:	BLFLLBZGZJTVJG-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	165.19
CAS:	94-09-7

Physical Properties

Property code	Value	Unit	Source
chs	-4694.90 ± 0.80	kJ/mol	NIST Webbook
chs	-4697.80 ± 0.80	kJ/mol	NIST Webbook
gf	-39.79	kJ/mol	Joback Method
hf	-215.04	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-2.74		Aqueous Solubility Prediction Method
log10ws	-2.10		Estimated Solubility Method
log10ws	-2.62		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.16		Aqueous Solubility Prediction Method
logp	1.446		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1535.00		NIST Webbook

rinpol	1555.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	585.80	K	Joback Method
tc	812.12	K	Joback Method
tf	344.15 ± 1.00	K	NIST Webbook
tf	363.00 ± 1.00	K	NIST Webbook
tf	362.00 ± 1.00	K	NIST Webbook
tf	363.00 ± 0.50	K	NIST Webbook
tf	363.00 ± 0.50	K	NIST Webbook
tf	362.90	K	Aqueous Solubility Prediction Method
tf	362.90	K	Aqueous Solubility Prediction Method
tf	362.70 ± 0.50	K	NIST Webbook
tt	363.20	K	Solubility of Ethyl p-Aminobenzoate in Six Alcohols within (283.15 to 327.15) K
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.54	J/mol×K	736.68	Joback Method
cpg	363.84	J/mol×K	774.40	Joback Method
cpg	310.15	J/mol×K	585.80	Joback Method
cpg	322.35	J/mol×K	623.52	Joback Method
cpg	333.81	J/mol×K	661.24	Joback Method
cpg	344.53	J/mol×K	698.96	Joback Method
cpg	372.45	J/mol×K	812.12	Joback Method
hfust	24.60	kJ/mol	362.60	NIST Webbook

hfust	23.56	kJ/mol	362.80	NIST Webbook

Sources

Single-component and mixture solubilities of ethyl p-hydroxybenzoate and ethyl p-aminobenzoate in supercritical CO2:	https://www.doi.org/10.1016/j.fluid.2007.09.020
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
Solubility of Ethyl p-Aminobenzoate in Six Alcohols within (283.15 to 327.15) K:	https://www.doi.org/10.1021/acs.jced.6b00037
The Solubility of Benzocaine, Lidocaine, and Procaine in Liquid and Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je034163p
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of the Drugs Benzocaine, Metronidazole Benzoate, and Naproxen in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je020218w
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
tt:	Triple Point Temperature
vc:	Critical Volume

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