Procaine

Other names: .beta.-(diethylamino)ethyl p-aminobenzoate
.beta.-diethylaminoethyl 4-aminobenzoate
2-(Diethylamino)ethyl 4-aminobenzoate
2-(Diethylamino)ethyl p-aminobenzoate
2-Diethylaminoethyl 4-aminobenzoate
2-Diethylaminoethylester kyseliny p-aminobenzoove
4-Aminobenzoic acid diethylaminoethyl ester
Benzoic acid, 4-amino-, 2-(diethylamino)ethyl ester
Benzoic acid, p-amino-, 2-(diethylamino)ethyl ester
Diethylaminoethyl p-aminobenzoate
Duracaine
NSC 169497
Nissocaine
Procain
Spinocaine
Vitamin H3
benzoic acid, p-amino-, 2-(diethylamino) ethyl ester
p-Aminobenzoic acid, 2-(diethylamino)ethyl ester
p-Aminobenzoyldiethylaminoethanol
p-aminobenzoic acid 2-diethylaminoethyl ester
procaine base
«beta»-(Diethylamino)ethyl 4-aminobenzoate
«beta»-(Diethylamino)ethyl p-aminobenzoate
Â«betaÂ»-(Diethylamino)ethyl 4-aminobenzoate
Â«betaÂ»-(Diethylamino)ethyl p-aminobenzoate

Inchi: InChI=1S/C13H20N2O2/c1-3-15(4-2)9-10-17-13(16)11-5-7-12(14)8-6-11/h5-8H,3-4,9-10
InchiKey: MFDFERRIHVXMIY-UHFFFAOYSA-N
Formula: C13H20N2O2
SMILES: CCN(CC)CCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 236.31
CAS: 59-46-1

Physical Properties

Property code	Value	Unit	Source
gf	104.67	kJ/mol	Joback Method
hf	-230.07	kJ/mol	Joback Method

hfus	34.08	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-1.50		Aqueous Solubility Prediction Method
logp	1.767		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	1979.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2035.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook

rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
ripol	3250.00		NIST Webbook
ripol	3250.00		NIST Webbook
tb	689.76	K	Joback Method
tc	898.32	K	Joback Method
tf	463.10	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.04	J/mol×K	689.76	Joback Method
cpg	561.16	J/mol×K	724.52	Joback Method
cpg	575.33	J/mol×K	759.28	Joback Method
cpg	588.58	J/mol×K	794.04	Joback Method
cpg	600.94	J/mol×K	828.80	Joback Method
cpg	612.45	J/mol×K	863.56	Joback Method
cpg	623.13	J/mol×K	898.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59461&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Solubility of Benzocaine, Lidocaine, and Procaine in Liquid and Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je034163p

Thermodynamic Study of the Solubility of Procaine HCl in Some Ethanol + Water Cosolvent Mixtures: https://www.doi.org/10.1021/je900958z

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume