

Procainamide

Other names:

Benzamide, 4-amino-N-[2-(diethylamino)ethyl]-
Benzamide, p-amino-N-[2-(diethylamino)ethyl]-
p-Amino-N-(2-diethylaminoethyl)benzamide
p-Aminobenzoic diethylaminoethylamide
Novocainamid
Novocainamide
Novocaine amide
Novocamid
Procaine amide
Procamide
Biocoryl
Procapan (free base)
Pronestyl
2-Diethylaminoethylamid kyseliny p-aminobenzoove
4-Amino-N-(diethylaminoethyl)benzamide
NSC 27461

Inchi:

InChI=1S/C13H21N3O/c1-3-16(4-2)10-9-15-13(17)11-5-7-12(14)8-6-11/h5-8H,3-4,9-10,1

InchiKey:

REQCZEXYDRLIBE-UHFFFAOYSA-N

Formula:

C13H21N3O

SMILES:

CCN(CC)CCNC(=O)c1ccc(N)cc1

Mol. weight [g/mol]:

235.33

CAS:

51-06-9

Physical Properties

Property code	Value	Unit	Source
gf	299.06	kJ/mol	Joback Method
hf	-44.38	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.340		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2248.00		NIST Webbook

rinpol	2193.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	717.51	K	Joback Method
tc	927.86	K	Joback Method
tf	493.53	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.45	J/mol×K	717.51	Joback Method
cpg	588.30	J/mol×K	752.57	Joback Method
cpg	602.18	J/mol×K	787.63	Joback Method
cpg	615.14	J/mol×K	822.69	Joback Method
cpg	627.23	J/mol×K	857.75	Joback Method
cpg	638.49	J/mol×K	892.80	Joback Method
cpg	648.98	J/mol×K	927.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51069&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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