Lidocaine

Other names:

2',6'-Acetoxylidide, 2-(diethylamino)-
2-(Diethylamino)-2',6'-acetoxylidide
2-(diethylamino)-N-(2,6-dimethylphenyl)acetamide
2-diethylamino-N-(2,6-dimethylphenyl)acetamide
Acetamide, 2-(diethylamino)-N-(2,6-dimethylphenyl)-
Anbesol
Anestacon
Cappicaine
Cito optadren
Cuivasil
Dalcaine
Diethylaminoacet-2,6-xylidide
Diethylaminoaceto-2,6-xylidide
Duncaine
ELA-Max
Esracaine
Gravocain
Isicaina
Isicaine
Jetocaine
L-Caine
Leostesin
Lida-Mantle
Lidoderm
Lignocaine
Maricaine
Remicaine
Rucaina
Solarcaine
Solcain
Xilina
Xilocaina
Xycaine
Xylestesin
Xyline
Xylocain
Xylocaine
Xylocitin
Xyloneural (free base)
Xylotox

alfa-Dietilamino-2,6-dimetilacetanilide
«alpha»-(Diethylamino)-2,6-acetoxylidide
«alpha»-Diethylamino-2,6-dimethylacetanilide
«alpha»-Diethylaminoaceto-2,6-xylidide
«omega»-Diethylamino-2,6-dimethylacetanilide
Â«alphaÂ»-(Diethylamino)-2,6-acetoxylidide
Â«alphaÂ»-Diethylamino-2,6-dimethylacetanilide
Â«alphaÂ»-Diethylaminoaceto-2,6-xylidide
Â«omegaÂ»-Diethylamino-2,6-dimethylacetanilide

Inchi: InChI=1S/C14H22N2O/c1-5-16(6-2)10-13(17)15-14-11(3)8-7-9-12(14)4/h7-9H,5-6,10H2,

InchiKey: NNJVILVZKWQKPM-UHFFFAOYSA-N

Formula: C14H22N2O

SMILES: CCN(CC)CC(=O)Nc1c(C)cccc1C

Mol. weight [g/mol]: 234.34

CAS: 137-58-6

Physical Properties

Property code	Value	Unit	Source
gf	231.40	kJ/mol	Joback Method
hf	-110.28	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-1.77		Aqueous Solubility Prediction Method
log10ws	-1.87		Aqueous Solubility Prediction Method
logp	2.584		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1881.00		NIST Webbook

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rinpol	1859.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	672.84	K	Joback Method
tc	874.39	K	Joback Method
tf	341.65	K	Aqueous Solubility Prediction Method
tf	341.65	K	Aqueous Solubility Prediction Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.04	J/mol×K	807.20	Joback Method
cpg	631.58	J/mol×K	840.79	Joback Method
cpg	560.26	J/mol×K	672.84	Joback Method
cpg	576.33	J/mol×K	706.43	Joback Method
cpg	591.46	J/mol×K	740.02	Joback Method
cpg	605.68	J/mol×K	773.61	Joback Method
cpg	643.32	J/mol×K	874.39	Joback Method
hfust	16.40	kJ/mol	340.70	NIST Webbook
hfust	18.80	kJ/mol	341.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.20	K	0.50	NIST Webbook

Sources

Thermodynamic properties of hydrophobic deep eutectic solvents https://www.doi.org/10.1016/j.fluid.2019.02.010

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

and Solubility of Water and HMF in Binary Mixtures and PC-SAFT Modeling:

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

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137586&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume