2-DIETHYLAMINO-N-(2,6-XYLYL)ACETAMIDE

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
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
acetamide, 2-(diethylamino)-N-(2,6-dimethylphenyl)-

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

Physical Properties

Property code	Value	Unit	Source
hfus	35.00	kJ/mol	Joback Method
ie	7.39	eV	Cheméo Relay (1.0)
log10ws	-1.87		Aqueous Solubility Prediction Method
log10ws	-1.77		Aqueous Solubility Prediction Method
logp	2.584		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1885.00		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
rinpol	1890.00		NIST Webbook
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rinpol	1882.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1859.00		NIST Webbook
tf	341.65	K	Aqueous Solubility Prediction Method
tf	341.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	619.04	J/mol×K	807.20	Joback Method
cpg	631.58	J/mol×K	840.79	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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137586&Units=SI

Interpretation of the global heat of melting in eutectic binary systems: https://www.doi.org/10.1016/j.tca.2018.04.011

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermodynamic properties of hydrophobic deep eutectic solvents and solubility of water and HMF in them: Measurements and PC-SAFT modeling: https://www.doi.org/10.1016/j.fluid.2019.02.010

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

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point