

4-DODECYLANILINE

Other names:	4-n-Dodecylamine Benzenamine, 4-dodecyl- p-Dodecylaniline
Inchi:	InChI=1S/C18H31N/c1-2-3-4-5-6-7-8-9-10-11-12-17-13-15-18(19)16-14-17/h13-16H,2-12H
InchiKey:	KLPPPIIEMUEGP-UHFFFAOYSA-N
Formula:	C18H31N
SMILES:	CCCCCCCCCCCCc1ccc(N)cc1
Mol. weight [g/mol]:	261.45

Physical Properties

Property code	Value	Unit	Source
af	0.8812		Cheméo Relay (1.0)
gf	269.91	kJ/mol	Joback Method
hf	-176.85	kJ/mol	Cheméo Relay (1.0)
hfus	41.22	kJ/mol	Joback Method
hvap	102.66	kJ/mol	Cheméo Relay (1.0)
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-6.33		Cheméo Relay (1.0)
logp	5.732		Crippen Method
mcvol	250.700	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
tb	634.99	K	Cheméo Relay (1.0)
tc	826.81	K	Cheméo Relay (1.0)
tf	312.62	K	Cheméo Relay (1.0)
vc	0.955	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.50	J/mol×K	715.43	Joback Method
cpg	749.07	J/mol×K	747.85	Joback Method
cpg	766.63	J/mol×K	780.26	Joback Method
cpg	783.22	J/mol×K	812.68	Joback Method
cpg	798.89	J/mol×K	845.09	Joback Method

cpg	813.68	J/mol×K	877.51	Joback Method
cpg	827.63	J/mol×K	909.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104427&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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