4-Dodecylaniline

Other names: p-Dodecylaniline
4-n-Dodecylamine
Benzenamine, 4-dodecyl-
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,2-12
InchiKey: KLPPPIIIEMUEGP-UHFFFAOYSA-N
Formula: C18H31N
SMILES: CCCCCCCCCCCCc1ccc(N)cc1
Mol. weight [g/mol]: 261.45
CAS: 104-42-7

Physical Properties

Property code	Value	Unit	Source
gf	269.91	kJ/mol	Joback Method
hf	-156.00	kJ/mol	Joback Method
hfus	41.22	kJ/mol	Joback Method
hvap	69.24	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.732		Crippen Method
mcvol	250.700	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
tb	715.43	K	Joback Method
tc	909.93	K	Joback Method
tf	414.82	K	Joback Method
vc	0.965	m3/kmol	Joback Method

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