Benzenamine, N-dodecyl-

Other names: N-Dodecylaniline
Inchi: InChI=1S/C18H31N/c1-2-3-4-5-6-7-8-9-10-14-17-19-18-15-12-11-13-16-18/h11-13,15-16
InchiKey: LQKYCMRSWKQVBQ-UHFFFAOYSA-N
Formula: C18H31N
SMILES: CCCCCCCCCCCCNc1ccccc1
Mol. weight [g/mol]: 261.45
CAS: 3007-74-7

Physical Properties

Property code	Value	Unit	Source
gf	302.48	kJ/mol	Joback Method
hf	-124.85	kJ/mol	Joback Method
hfus	41.52	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
log10ws	-6.08		Crippen Method
logp	6.019		Crippen Method
mcvol	250.700	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
tb	688.09	K	Joback Method
tc	875.50	K	Joback Method
tf	371.70	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.55	J/mol×K	688.09	Joback Method
cpg	735.58	J/mol×K	719.33	Joback Method
cpg	753.59	J/mol×K	750.56	Joback Method
cpg	770.64	J/mol×K	781.80	Joback Method
cpg	786.76	J/mol×K	813.03	Joback Method
cpg	802.00	J/mol×K	844.27	Joback Method
cpg	816.40	J/mol×K	875.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3007747&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
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