

Aniline, n-octyl-

Other names:	N-Octylaniline
Inchi:	InChI=1S/C14H23N/c1-2-3-4-5-6-10-13-15-14-11-8-7-9-12-14/h7-9,11-12,15H,2-6,10,13
InchiKey:	GCULWAWIZUGXTO-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCCCCCNc1cccc1
Mol. weight [g/mol]:	205.34
CAS:	3007-71-4

Physical Properties

Property code	Value	Unit	Source
gf	268.80	kJ/mol	Joback Method
hf	-42.29	kJ/mol	Joback Method
hfus	31.16	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
log10ws	-4.41		Crippen Method
logp	4.459		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	596.57	K	Joback Method
tc	791.57	K	Joback Method
tf	326.62	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.81	J/molxK	596.57	Joback Method
cpg	516.51	J/molxK	629.07	Joback Method
cpg	533.25	J/molxK	661.57	Joback Method
cpg	549.07	J/molxK	694.07	Joback Method
cpg	564.00	J/molxK	726.57	Joback Method
cpg	578.08	J/molxK	759.07	Joback Method
cpg	591.36	J/molxK	791.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3007714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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