4-Octylaniline

Other names:	p-Octylaniline
	4-n-Octylaniline
	Benzenamine, 4-octyl-
	4-(n-C8H17)C6H4NH2
Inchi:	InChI=1S/C14H23N/c1-2-3-4-5-6-7-8-13-9-11-14(15)12-10-13/h9-12H,2-8,15H2,1H3
InchiKey:	ORKQJTBYQZITLA-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCCCCCc1ccc(N)cc1
Mol. weight [g/mol]:	205.34
CAS:	16245-79-7

Physical Properties

Property code	Value	Unit	Source
affp	894.50	kJ/mol	NIST Webbook
basg	862.00	kJ/mol	NIST Webbook
gf	236.23	kJ/mol	Joback Method
hf	-73.44	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.172		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
tb	623.91	K	Joback Method
tc	827.35	K	Joback Method
tf	369.74	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.92	J/mol×K	623.91	Joback Method
cpg	529.14	J/mol×K	657.82	Joback Method
cpg	545.40	J/mol×K	691.72	Joback Method

cpg	560.74	J/mol×K	725.63	Joback Method
cpg	575.21	J/mol×K	759.54	Joback Method
cpg	588.84	J/mol×K	793.44	Joback Method
cpg	601.66	J/mol×K	827.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	1.70	NIST Webbook
tbrp	456.50 ± 1.50	K	2.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16245797&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume