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]:	205.35

Physical Properties

Property code	Value	Unit	Source
af	0.7369		Cheméo Relay (1.0)
affp	894.50	kJ/mol	NIST Webbook
basg	862.00	kJ/mol	NIST Webbook
gf	236.23	kJ/mol	Joback Method
hf	-90.91	kJ/mol	Cheméo Relay (1.0)
hfus	30.87	kJ/mol	Joback Method
hvap	83.45	kJ/mol	Cheméo Relay (1.0)
ie	7.65	eV	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	4.172		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
tb	593.79	K	Cheméo Relay (1.0)
tc	790.54	K	Cheméo Relay (1.0)
tf	291.96	K	Cheméo Relay (1.0)
vc	0.730	m3/kmol	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16245797&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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