

N,N-Dioctylaniline

Inchi:	InChI=1S/C22H39N/c1-3-5-7-9-11-16-20-23(22-18-14-13-15-19-22)21-17-12-10-8-6-4-2/
InchiKey:	PTRSTXBRQVXIEW-UHFFFAOYSA-N
Formula:	C22H39N
SMILES:	CCCCCCCCN(CCCCCCCC)c1ccccc1
Mol. weight [g/mol]:	317.55
CAS:	3007-75-8

Physical Properties

Property code	Value	Unit	Source
gf	357.55	kJ/mol	Joback Method
hf	-193.35	kJ/mol	Joback Method
hfus	49.80	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
ie	7.10	eV	NIST Webbook
log10ws	-7.24		Crippen Method
logp	7.214		Crippen Method
mcvol	307.060	ml/mol	McGowan Method
pc	1110.37	kPa	Joback Method
tb	741.88	K	Joback Method
tc	923.89	K	Joback Method
tf	396.59	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.32	J/molxK	741.88	Joback Method
cpg	949.07	J/molxK	772.21	Joback Method
cpg	968.74	J/molxK	802.55	Joback Method
cpg	987.37	J/molxK	832.88	Joback Method
cpg	1005.02	J/molxK	863.22	Joback Method
cpg	1021.74	J/molxK	893.55	Joback Method
cpg	1037.59	J/molxK	923.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3007758&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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