

2-Chloro-4-nitro-N,N-dipropylaniline

Other names:	4-Nitro-2-chloro-N,N-di-n-propyl aniline
Inchi:	InChI=1S/C12H17ClN2O2/c1-3-7-14(8-4-2)12-6-5-10(15(16)17)9-11(12)13/h5-6,9H,3-4,7
InchiKey:	OYJJPFCCGGNTTTO-UHFFFAOYSA-N
Formula:	C12H17ClN2O2
SMILES:	CCCN(CCC)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	256.73
CAS:	6216-91-7

Physical Properties

Property code	Value	Unit	Source
gf	277.71	kJ/mol	Joback Method
hf	-36.39	kJ/mol	Joback Method
hfus	38.68	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.875		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
tb	712.31	K	Joback Method
tc	938.29	K	Joback Method
tf	482.46	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.54	J/molxK	712.31	Joback Method
cpg	534.69	J/molxK	749.97	Joback Method
cpg	547.87	J/molxK	787.64	Joback Method
cpg	560.11	J/molxK	825.30	Joback Method
cpg	571.47	J/molxK	862.96	Joback Method
cpg	582.02	J/molxK	900.63	Joback Method
cpg	591.81	J/molxK	938.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.50 ± 0.50	K	0.09	NIST Webbook

Sources

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=C6216917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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