

N-Ethyl-p-chloro-amphetamine

Other names:	N-Ethyl-p-chloramphetamine Ethyl-p-chloramphetamine
Inchi:	InChI=1S/C11H16ClN/c1-3-13-9(2)8-10-4-6-11(12)7-5-10/h4-7,9,13H,3,8H2,1-2H3
InchiKey:	PRKDJWMNZDSUPT-UHFFFAOYSA-N
Formula:	C11H16ClN
SMILES:	CCNC(C)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	197.70

Physical Properties

Property code	Value	Unit	Source
gf	219.54	kJ/mol	Joback Method
hf	-12.86	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.880		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1456.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	569.90	K	Joback Method
tc	783.28	K	Joback Method
tf	320.25	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.16	J/mol×K	569.90	Joback Method

cpg	395.29	J/mol×K	605.46	Joback Method
cpg	409.53	J/mol×K	641.03	Joback Method
cpg	422.89	J/mol×K	676.59	Joback Method
cpg	435.42	J/mol×K	712.15	Joback Method
cpg	447.16	J/mol×K	747.71	Joback Method
cpg	458.15	J/mol×K	783.28	Joback Method

Sources

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=R18151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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