

Benzamide, 4-chloro-N-ethyl-N-propyl-

Inchi:	InChI=1S/C12H16ClNO/c1-3-9-14(4-2)12(15)10-5-7-11(13)8-6-10/h5-8H,3-4,9H2,1-2H3
InchiKey:	NQGVDIATGHGYFO-UHFFFAOYSA-N
Formula:	C12H16ClNO
SMILES:	CCCN(CC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	225.72

Physical Properties

Property code	Value	Unit	Source
gf	122.87	kJ/mol	Joback Method
hf	-126.74	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.212		Crippen Method
mvol	179.970	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	609.36	K	Joback Method
tc	819.61	K	Joback Method
tf	376.26	K	Joback Method
vc	0.672	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.86	J/mol×K	609.36	Joback Method
cpg	447.62	J/mol×K	644.40	Joback Method
cpg	461.44	J/mol×K	679.44	Joback Method
cpg	474.38	J/mol×K	714.49	Joback Method
cpg	486.47	J/mol×K	749.53	Joback Method
cpg	497.76	J/mol×K	784.57	Joback Method
cpg	508.29	J/mol×K	819.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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