Benzamide, 4-chloro-N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C14H20ClNO/c1-4-16(10-9-11(2)3)14(17)12-5-7-13(15)8-6-12/h5-8,11H,4,9-10
InchiKey: ZVWWWTVLUNWQDP-UHFFFAOYSA-N
Formula: C14H20ClNO
SMILES: CCN(CCC(C)C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 253.77

Physical Properties

Property code	Value	Unit	Source
gf	137.27	kJ/mol	Joback Method
hf	-173.30	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	62.48	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.848		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	654.68	K	Joback Method
tc	862.49	K	Joback Method
tf	383.80	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.07	J/mol×K	654.68	Joback Method
cpg	551.14	J/mol×K	689.31	Joback Method
cpg	566.20	J/mol×K	723.95	Joback Method
cpg	580.30	J/mol×K	758.58	Joback Method
cpg	593.49	J/mol×K	793.22	Joback Method
cpg	605.81	J/mol×K	827.85	Joback Method
cpg	617.32	J/mol×K	862.49	Joback Method

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=U415324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume