Benzamide, 4-chloro-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C13H18ClNO/c1-4-15(9-10(2)3)13(16)11-5-7-12(14)8-6-11/h5-8,10H,4,9H2,1-3
InchiKey: JXLCZJMOWDMOSZ-UHFFFAOYSA-N
Formula: C13H18ClNO
SMILES: CCN(CC(C)C)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 239.74

Physical Properties

Property code	Value	Unit	Source
gf	128.85	kJ/mol	Joback Method
hf	-152.66	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.458		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	631.80	K	Joback Method
tc	842.83	K	Joback Method
tf	372.53	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.47	J/mol×K	631.80	Joback Method
cpg	499.10	J/mol×K	666.97	Joback Method
cpg	513.74	J/mol×K	702.14	Joback Method
cpg	527.42	J/mol×K	737.31	Joback Method
cpg	540.20	J/mol×K	772.48	Joback Method
cpg	552.13	J/mol×K	807.65	Joback Method
cpg	563.25	J/mol×K	842.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U415322&Units=SI

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