Benzamide, 4-chloro-N-ethyl-N-butyl-

Inchi: InChI=1S/C13H18ClNO/c1-3-5-10-15(4-2)13(16)11-6-8-12(14)9-7-11/h6-9H,3-5,10H2,1-2

InchiKey: CKVXMCCRBQYGDV-UHFFFAOYSA-N

Formula: C13H18ClNO

SMILES: CCCCN(CC)C(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 239.74

Physical Properties

Property code	Value	Unit	Source
gf	131.29	kJ/mol	Joback Method
hf	-147.38	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	60.64	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.602		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	632.24	K	Joback Method
tc	839.24	K	Joback Method
tf	387.53	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.02	J/mol×K	632.24	Joback Method
cpg	498.31	J/mol×K	666.74	Joback Method
cpg	512.65	J/mol×K	701.24	Joback Method
cpg	526.09	J/mol×K	735.74	Joback Method
cpg	538.66	J/mol×K	770.24	Joback Method
cpg	550.42	J/mol×K	804.74	Joback Method
cpg	561.41	J/mol×K	839.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415323&Units=SI
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

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