Cyclopentanecarboxamide, N-butyl-N-isobutyl-

Inchi: InChI=1S/C14H27NO/c1-4-5-10-15(11-12(2)3)14(16)13-8-6-7-9-13/h12-13H,4-11H2,1-3H

InchiKey: WCYABKBLHPHKAD-UHFFFAOYSA-N

Formula: C14H27NO

SMILES: CCCCN(CC(C)C)C(=O)C1CCCC1

Mol. weight [g/mol]: 225.37

Physical Properties

Property code	Value	Unit	Source
gf	82.97	kJ/mol	Joback Method
hf	-322.14	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.461		Crippen Method
mcvol	208.810	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	600.87	K	Joback Method
tc	792.00	K	Joback Method
tf	325.84	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.34	J/mol×K	600.87	Joback Method
cpg	587.55	J/mol×K	632.72	Joback Method
cpg	606.67	J/mol×K	664.58	Joback Method
cpg	624.74	J/mol×K	696.43	Joback Method
cpg	641.80	J/mol×K	728.29	Joback Method
cpg	657.89	J/mol×K	760.14	Joback Method
cpg	673.06	J/mol×K	792.00	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=U415625&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