Cyclopentanecarboxamide, N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C15H29NO/c1-4-5-11-16(12-10-13(2)3)15(17)14-8-6-7-9-14/h13-14H,4-12H2,1

InchiKey: URJQCUFVACPLFW-UHFFFAOYSA-N

Formula: C15H29NO

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

Mol. weight [g/mol]: 239.40

Physical Properties

Property code	Value	Unit	Source
gf	91.39	kJ/mol	Joback Method
hf	-342.78	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.851		Crippen Method
mcvol	222.900	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	623.75	K	Joback Method
tc	812.77	K	Joback Method
tf	337.11	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.04	J/mol×K	623.75	Joback Method
cpg	642.51	J/mol×K	655.25	Joback Method
cpg	661.89	J/mol×K	686.76	Joback Method
cpg	680.20	J/mol×K	718.26	Joback Method
cpg	697.50	J/mol×K	749.77	Joback Method
cpg	713.83	J/mol×K	781.27	Joback Method
cpg	729.24	J/mol×K	812.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415627&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