

Cyclopentanecarboxamide, N,N-dibutyl-

Inchi:	InChI=1S/C14H27NO/c1-3-5-11-15(12-6-4-2)14(16)13-9-7-8-10-13/h13H,3-12H2,1-2H3
InchiKey:	UPXNABGIFBROJI-UHFFFAOYSA-N
Formula:	C14H27NO
SMILES:	CCCCN(CCCC)C(=O)C1CCCC1
Mol. weight [g/mol]:	225.37

Physical Properties

Property code	Value	Unit	Source
gf	85.41	kJ/mol	Joback Method
hf	-316.86	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.605		Crippen Method
mvol	208.810	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	601.31	K	Joback Method
tc	788.97	K	Joback Method
tf	340.84	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.01	J/mol×K	601.31	Joback Method
cpg	586.81	J/mol×K	632.59	Joback Method
cpg	605.56	J/mol×K	663.86	Joback Method
cpg	623.30	J/mol×K	695.14	Joback Method
cpg	640.08	J/mol×K	726.42	Joback Method
cpg	655.94	J/mol×K	757.69	Joback Method
cpg	670.91	J/mol×K	788.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308608&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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