Cyclopentanecarboxamide, N-butyl-N-pentyl-

Inchi: InChI=1S/C15H29NO/c1-3-5-9-13-16(12-6-4-2)15(17)14-10-7-8-11-14/h14H,3-13H2,1-2H
InchiKey: PGXQSBKNJCKRDR-UHFFFAOYSA-N
Formula: C15H29NO
SMILES: CCCCCN(CCCC)C(=O)C1CCCC1
Mol. weight [g/mol]: 239.40

Physical Properties

Property code	Value	Unit	Source
gf	93.83	kJ/mol	Joback Method
hf	-337.50	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	58.03	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.996		Crippen Method
mcvol	222.900	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook
tb	624.19	K	Joback Method
tc	809.98	K	Joback Method
tf	352.11	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.69	J/mol×K	624.19	Joback Method
cpg	641.77	J/mol×K	655.15	Joback Method
cpg	660.79	J/mol×K	686.12	Joback Method
cpg	678.80	J/mol×K	717.08	Joback Method
cpg	695.84	J/mol×K	748.05	Joback Method
cpg	711.94	J/mol×K	779.01	Joback Method
cpg	727.16	J/mol×K	809.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415628&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

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

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