Cyclopentanecarboxamide, N-butyl-N-hexyl-

Inchi: InChI=1S/C16H31NO/c1-3-5-7-10-14-17(13-6-4-2)16(18)15-11-8-9-12-15/h15H,3-14H2,1
InchiKey: KSJSKOFHNIBSMO-UHFFFAOYSA-N
Formula: C16H31NO
SMILES: CCCCCCN(CCCC)C(=O)C1CCCC1
Mol. weight [g/mol]: 253.42

Physical Properties

Property code	Value	Unit	Source
gf	102.25	kJ/mol	Joback Method
hf	-358.14	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.386		Crippen Method
mcvol	236.990	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	2209.00		NIST Webbook
rinpol	2209.00		NIST Webbook
tb	647.07	K	Joback Method
tc	831.29	K	Joback Method
tf	363.38	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.64	J/mol×K	647.07	Joback Method
cpg	697.96	J/mol×K	677.77	Joback Method
cpg	717.22	J/mol×K	708.48	Joback Method
cpg	735.45	J/mol×K	739.18	Joback Method
cpg	752.71	J/mol×K	769.89	Joback Method
cpg	769.02	J/mol×K	800.59	Joback Method
cpg	784.44	J/mol×K	831.29	Joback Method

Sources

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=U415630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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