

Cyclopentanecarboxamide, N-butyl-N-nonyl-

Inchi:

InChI=1S/C19H37NO/c1-3-5-7-8-9-10-13-17-20(16-6-4-2)19(21)18-14-11-12-15-18/h18H

InchiKey:

ICTXDZGLUDJPFM-UHFFFAOYSA-N

Formula:

C19H37NO

SMILES:

CCCCCCCCCN(CCCC)C(=O)C1CCCC1

Mol. weight [g/mol]:

295.50

Physical Properties

Property code	Value	Unit	Source
gf	127.51	kJ/mol	Joback Method
hf	-420.06	kJ/mol	Joback Method
hfus	43.52	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.556		Crippen Method
mcvol	279.260	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	715.71	K	Joback Method
tc	897.55	K	Joback Method
tf	397.19	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.35	J/mol×K	715.71	Joback Method
cpg	873.26	J/mol×K	746.02	Joback Method
cpg	893.08	J/mol×K	776.32	Joback Method
cpg	911.84	J/mol×K	806.63	Joback Method
cpg	929.60	J/mol×K	836.94	Joback Method
cpg	946.40	J/mol×K	867.25	Joback Method
cpg	962.29	J/mol×K	897.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415634&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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