Cyclopentanecarboxamide, N-butyl-N-octyl-

Inchi: InChI=1S/C18H35NO/c1-3-5-7-8-9-12-16-19(15-6-4-2)18(20)17-13-10-11-14-17/h17H,3-
InchiKey: ZKJYOXQFGQPZAF-UHFFFAOYSA-N
Formula: C18H35NO
SMILES: CCCCCCCCN(CCCC)C(=O)C1CCCC1
Mol. weight [g/mol]: 281.48

Physical Properties

Property code	Value	Unit	Source
gf	119.09	kJ/mol	Joback Method
hf	-399.42	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	64.71	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.166		Crippen Method
mcvol	265.170	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	692.83	K	Joback Method
tc	875.03	K	Joback Method
tf	385.92	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.05	J/mol×K	692.83	Joback Method
cpg	813.77	J/mol×K	723.20	Joback Method
cpg	833.42	J/mol×K	753.56	Joback Method
cpg	852.02	J/mol×K	783.93	Joback Method
cpg	869.62	J/mol×K	814.30	Joback Method
cpg	886.28	J/mol×K	844.66	Joback Method
cpg	902.03	J/mol×K	875.03	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=U415633&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume