Cyclopentanecarboxamide, N-butyl-N-2-ethylhexyl-

Inchi: InChI=1S/C18H35NO/c1-4-7-11-16(6-3)15-19(14-8-5-2)18(20)17-12-9-10-13-17/h16-17H

InchiKey: LICRYVGEVHVZHM-UHFFFAOYSA-N

Formula: C18H35NO

SMILES: CCCCC(CC)CN(CCCC)C(=O)C1CCCC1

Mol. weight [g/mol]: 281.48

Physical Properties

Property code	Value	Unit	Source
gf	116.65	kJ/mol	Joback Method
hf	-404.70	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	5.022		Crippen Method
mcvol	265.170	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	692.39	K	Joback Method
tc	877.09	K	Joback Method
tf	370.92	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.45	J/mol×K	692.39	Joback Method
cpg	814.49	J/mol×K	723.17	Joback Method
cpg	834.41	J/mol×K	753.96	Joback Method
cpg	853.25	J/mol×K	784.74	Joback Method
cpg	871.06	J/mol×K	815.52	Joback Method
cpg	887.89	J/mol×K	846.31	Joback Method
cpg	903.78	J/mol×K	877.09	Joback Method

Sources

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=U415631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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