Cyclopentanecarboxamide, N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C17H33NO/c1-4-6-8-11-15(3)18(14-7-5-2)17(19)16-12-9-10-13-16/h15-16H,4-

InchiKey: YPFSDSUBTRMYQX-UHFFFAOYSA-N

Formula: C17H33NO

SMILES: CCCCCC(C)N(CCCC)C(=O)C1CCCC1

Mol. weight [g/mol]: 267.45

Physical Properties

Property code	Value	Unit	Source
gf	108.23	kJ/mol	Joback Method
hf	-384.06	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.774		Crippen Method
mcvol	251.080	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	669.51	K	Joback Method
tc	855.27	K	Joback Method
tf	359.65	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.18	J/mol×K	669.51	Joback Method
cpg	756.05	J/mol×K	700.47	Joback Method
cpg	775.82	J/mol×K	731.43	Joback Method
cpg	794.51	J/mol×K	762.39	Joback Method
cpg	812.17	J/mol×K	793.35	Joback Method
cpg	828.86	J/mol×K	824.31	Joback Method
cpg	844.62	J/mol×K	855.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415629&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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