

Cyclopentanecarboxamide, N-butyl-N-undecyl-

Inchi: InChI=1S/C21H41NO/c1-3-5-7-8-9-10-11-12-15-19-22(18-6-4-2)21(23)20-16-13-14-17-2
InchiKey: SQXYXUXZJZHJX-UHFFFAOYSA-N
Formula: C21H41NO
SMILES: CCCCCCCCCCN(CCCC)C(=O)C1CCCC1
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	144.35	kJ/mol	Joback Method
hf	-461.34	kJ/mol	Joback Method
hfus	48.70	kJ/mol	Joback Method
hvap	71.39	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.336		Crippen Method
mcvol	307.440	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	3135.00		NIST Webbook
rinpol	3135.00		NIST Webbook
tb	761.47	K	Joback Method
tc	944.16	K	Joback Method
tf	419.73	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.78	J/mol×K	761.47	Joback Method
cpg	995.09	J/mol×K	791.92	Joback Method
cpg	1015.27	J/mol×K	822.37	Joback Method
cpg	1034.37	J/mol×K	852.82	Joback Method
cpg	1052.43	J/mol×K	883.26	Joback Method
cpg	1069.52	J/mol×K	913.71	Joback Method
cpg	1085.68	J/mol×K	944.16	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=U415636&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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