Cyclohexanecarboxamide, N,N-dihexyl-

Inchi: InChI=1S/C19H37NO/c1-3-5-7-12-16-20(17-13-8-6-4-2)19(21)18-14-10-9-11-15-18/h18H
InchiKey: MLUSCIXBFIUBJL-UHFFFAOYSA-N
Formula: C19H37NO
SMILES: CCCCCCN(CCCCCC)C(=O)C1CCCCC1
Mol. weight [g/mol]: 295.50

Physical Properties

Property code	Value	Unit	Source
gf	115.41	kJ/mol	Joback Method
hf	-426.22	kJ/mol	Joback Method
hfus	41.42	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.556		Crippen Method
mcvol	279.260	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	719.98	K	Joback Method
tc	905.81	K	Joback Method
tf	393.67	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.22	J/mol×K	719.98	Joback Method
cpg	877.74	J/mol×K	750.95	Joback Method
cpg	898.07	J/mol×K	781.92	Joback Method
cpg	917.27	J/mol×K	812.90	Joback Method
cpg	935.38	J/mol×K	843.87	Joback Method
cpg	952.44	J/mol×K	874.84	Joback Method
cpg	968.51	J/mol×K	905.81	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=U308521&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