Propanamide, N,N-dihexyl-3-cyclopentyl-

Inchi: InChI=1S/C20H39NO/c1-3-5-7-11-17-21(18-12-8-6-4-2)20(22)16-15-19-13-9-10-14-19/h1
InchiKey: BLBVBLUSZAQSEN-UHFFFAOYSA-N
Formula: C20H39NO
SMILES: CCCCCCN(CCCCCC)C(=O)CCC1CCCC1
Mol. weight [g/mol]: 309.53

Physical Properties

Property code	Value	Unit	Source
gf	135.93	kJ/mol	Joback Method
hf	-440.70	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.946		Crippen Method
mcvol	293.350	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	2276.00		NIST Webbook
tb	738.59	K	Joback Method
tc	920.58	K	Joback Method
tf	408.46	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.61	J/mol×K	738.59	Joback Method
cpg	933.72	J/mol×K	768.92	Joback Method
cpg	953.71	J/mol×K	799.25	Joback Method
cpg	972.64	J/mol×K	829.58	Joback Method
cpg	990.55	J/mol×K	859.92	Joback Method
cpg	1007.49	J/mol×K	890.25	Joback Method
cpg	1023.52	J/mol×K	920.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308281&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