Propanamide, N,N-diheptyl-3-cyclopentyl-

Inchi: InChI=1S/C22H43NO/c1-3-5-7-9-13-19-23(20-14-10-8-6-4-2)22(24)18-17-21-15-11-12-1
InchiKey: XEVNPAKTLRPCEN-UHFFFAOYSA-N
Formula: C22H43NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)CCC1CCCC1
Mol. weight [g/mol]: 337.58

Physical Properties

Property code	Value	Unit	Source
gf	152.77	kJ/mol	Joback Method
hf	-481.98	kJ/mol	Joback Method
hfus	51.29	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.726		Crippen Method
mcvol	321.530	ml/mol	McGowan Method
pc	1048.01	kPa	Joback Method
rinpol	2474.00		NIST Webbook
tb	784.35	K	Joback Method
tc	968.35	K	Joback Method
tf	431.00	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.78	J/mol×K	784.35	Joback Method
cpg	1057.33	J/mol×K	815.02	Joback Method
cpg	1077.71	J/mol×K	845.68	Joback Method
cpg	1096.99	J/mol×K	876.35	Joback Method
cpg	1115.23	J/mol×K	907.02	Joback Method
cpg	1132.47	J/mol×K	937.69	Joback Method
cpg	1148.77	J/mol×K	968.35	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=U308284&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume