Propanamide, N-heptyl-N-octyl-3-cyclopentyl-

Inchi: InChI=1S/C23H45NO/c1-3-5-7-9-11-15-21-24(20-14-10-8-6-4-2)23(25)19-18-22-16-12-13
InchiKey: AZYZBMIWWPUSMO-UHFFFAOYSA-N
Formula: C23H45NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CCC1CCCC1
Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	161.19	kJ/mol	Joback Method
hf	-502.62	kJ/mol	Joback Method
hfus	53.88	kJ/mol	Joback Method
hvap	75.84	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	7.116		Crippen Method
mcvol	335.620	ml/mol	McGowan Method
pc	985.78	kPa	Joback Method
rinpol	2573.00		NIST Webbook
tb	807.23	K	Joback Method
tc	993.21	K	Joback Method
tf	442.27	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.56	J/mol×K	807.23	Joback Method
cpg	1120.37	J/mol×K	838.23	Joback Method
cpg	1140.99	J/mol×K	869.22	Joback Method
cpg	1160.48	J/mol×K	900.22	Joback Method
cpg	1178.90	J/mol×K	931.22	Joback Method
cpg	1196.32	J/mol×K	962.21	Joback Method
cpg	1212.78	J/mol×K	993.21	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=U308285&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