Cyclohexanecarboxamide, N,N-diheptyl-

Inchi: InChI=1S/C21H41NO/c1-3-5-7-9-14-18-22(19-15-10-8-6-4-2)21(23)20-16-12-11-13-17-2(
InchiKey: TYJVMSHKYADCAZ-UHFFFAOYSA-N
Formula: C21H41NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C1CCCCC1
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	132.25	kJ/mol	Joback Method
hf	-467.50	kJ/mol	Joback Method
hfus	46.60	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.336		Crippen Method
mcvol	307.440	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	765.74	K	Joback Method
tc	951.68	K	Joback Method
tf	416.21	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.15	J/mol×K	765.74	Joback Method
cpg	999.92	J/mol×K	796.73	Joback Method
cpg	1020.47	J/mol×K	827.72	Joback Method
cpg	1039.86	J/mol×K	858.71	Joback Method
cpg	1058.13	J/mol×K	889.70	Joback Method
cpg	1075.34	J/mol×K	920.69	Joback Method
cpg	1091.53	J/mol×K	951.68	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=U308524&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