Cyclohexanecarboxamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C22H43NO/c1-3-5-7-9-11-16-20-23(19-15-10-8-6-4-2)22(24)21-17-13-12-14-18
InchiKey: ZDXRWYPNKWDLPT-UHFFFAOYSA-N
Formula: C22H43NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C1CCCCC1
Mol. weight [g/mol]: 337.58

Physical Properties

Property code	Value	Unit	Source
gf	140.67	kJ/mol	Joback Method
hf	-488.14	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.726		Crippen Method
mcvol	321.530	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	788.62	K	Joback Method
tc	975.49	K	Joback Method
tf	427.48	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.36	J/mol×K	788.62	Joback Method
cpg	1062.28	J/mol×K	819.77	Joback Method
cpg	1082.96	J/mol×K	850.91	Joback Method
cpg	1102.46	J/mol×K	882.06	Joback Method
cpg	1120.82	J/mol×K	913.20	Joback Method
cpg	1138.10	J/mol×K	944.35	Joback Method
cpg	1154.35	J/mol×K	975.49	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=U308525&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