Cyclohexanecarboxamide, N,N-diundecyl-

Inchi: InChI=1S/C29H57NO/c1-3-5-7-9-11-13-15-17-22-26-30(29(31)28-24-20-19-21-25-28)27-
InchiKey: YGERWCQDZWAOHT-UHFFFAOYSA-N
Formula: C29H57NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C1CCCCC1
Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	199.61	kJ/mol	Joback Method
hf	-632.62	kJ/mol	Joback Method
hfus	67.32	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.457		Crippen Method
mcvol	420.160	ml/mol	McGowan Method
pc	716.45	kPa	Joback Method
rinpol	3257.00		NIST Webbook
rinpol	3257.00		NIST Webbook
tb	948.78	K	Joback Method
tc	1163.94	K	Joback Method
tf	506.37	K	Joback Method
vc	1.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.41	J/mol×K	948.78	Joback Method
cpg	1517.69	J/mol×K	984.64	Joback Method
cpg	1540.35	J/mol×K	1020.50	Joback Method
cpg	1561.50	J/mol×K	1056.36	Joback Method
cpg	1581.23	J/mol×K	1092.22	Joback Method
cpg	1599.65	J/mol×K	1128.08	Joback Method
cpg	1616.86	J/mol×K	1163.94	Joback Method

Sources

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=U308529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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