

Cyclohexanecarboxamide, N,N-bis(2-ethylhexyl)-

Inchi: InChI=1S/C23H45NO/c1-5-9-14-20(7-3)18-24(19-21(8-4)15-10-6-2)23(25)22-16-12-11-1

InchiKey: LZMUWQUKBWZZGG-UHFFFAOYSA-N

Formula: C23H45NO

SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)C1CCCCC1

Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	144.21	kJ/mol	Joback Method
hf	-519.34	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.828		Crippen Method
mcvol	335.620	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2295.00		NIST Webbook
tb	810.62	K	Joback Method
tc	1001.75	K	Joback Method
tf	408.75	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.16	J/mol×K	810.62	Joback Method
cpg	1126.58	J/mol×K	842.48	Joback Method
cpg	1147.67	J/mol×K	874.33	Joback Method
cpg	1167.51	J/mol×K	906.19	Joback Method
cpg	1186.13	J/mol×K	938.04	Joback Method
cpg	1203.61	J/mol×K	969.90	Joback Method
cpg	1219.99	J/mol×K	1001.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308523&Units=SI
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

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

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