

Cyclobutanecarboxamide, N,N-dihexyl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H33NO/c1-3-5-7-9-14-18(15-10-8-6-4-2)17(19)16-12-11-13-16/h16H,3-15H2,17H

YDNRDDVTKFLGOD-UHFFFAOYSA-N

C17H33NO

CCCCCCN(CCCCCC)C(=O)C1CCC1

267.45

Physical Properties

Property code	Value	Unit	Source
gf	122.77	kJ/mol	Joback Method
hf	-372.62	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.776		Crippen Method
mcvol	251.080	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	665.68	K	Joback Method
tc	844.22	K	Joback Method
tf	378.17	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.59	J/mol×K	665.68	Joback Method
cpg	751.43	J/mol×K	695.44	Joback Method
cpg	770.27	J/mol×K	725.19	Joback Method
cpg	788.15	J/mol×K	754.95	Joback Method
cpg	805.12	J/mol×K	784.71	Joback Method
cpg	821.22	J/mol×K	814.46	Joback Method
cpg	836.51	J/mol×K	844.22	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=U308598&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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