

Cyclopropanecarboxamide, N,N-diheptyl-

Inchi:	InChI=1S/C18H35NO/c1-3-5-7-9-11-15-19(18(20)17-13-14-17)16-12-10-8-6-4-2/h17H,3-
InchiKey:	KPUGPQSLYZVGLK-UHFFFAOYSA-N
Formula:	C18H35NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)C1CC1
Mol. weight [g/mol]:	281.48

Physical Properties

Property code	Value	Unit	Source
gf	143.29	kJ/mol	Joback Method
hf	-387.10	kJ/mol	Joback Method
hfus	45.13	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.166		Crippen Method
mvol	265.170	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	684.29	K	Joback Method
tc	858.48	K	Joback Method
tf	392.96	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.10	J/mol×K	684.29	Joback Method
cpg	805.58	J/mol×K	713.32	Joback Method
cpg	824.11	J/mol×K	742.35	Joback Method
cpg	841.74	J/mol×K	771.39	Joback Method
cpg	858.52	J/mol×K	800.42	Joback Method
cpg	874.50	J/mol×K	829.45	Joback Method
cpg	889.72	J/mol×K	858.48	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=U308580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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