

Cyclopentanecarboxamide, N,N-diheptyl-

Inchi:	InChI=1S/C20H39NO/c1-3-5-7-9-13-17-21(18-14-10-8-6-4-2)20(22)19-15-11-12-16-19/h
InchiKey:	QWFSYNIKEZPUQR-UHFFFAOYSA-N
Formula:	C20H39NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)C1CCCC1
Mol. weight [g/mol]:	309.53

Physical Properties

Property code	Value	Unit	Source
gf	135.93	kJ/mol	Joback Method
hf	-440.70	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.946		Crippen Method
mcvol	293.350	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	2184.00		NIST Webbook
tb	738.59	K	Joback Method
tc	920.58	K	Joback Method
tf	408.46	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.61	J/mol×K	738.59	Joback Method
cpg	933.72	J/mol×K	768.92	Joback Method
cpg	953.71	J/mol×K	799.25	Joback Method
cpg	972.64	J/mol×K	829.58	Joback Method
cpg	990.55	J/mol×K	859.92	Joback Method
cpg	1007.49	J/mol×K	890.25	Joback Method
cpg	1023.52	J/mol×K	920.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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