

N,N'-Di-n-hexyladipamide

Inchi:	InChI=1S/C18H36N2O2/c1-3-5-7-11-15-19-17(21)13-9-10-14-18(22)20-16-12-8-6-4-2/h3
InchiKey:	BJRDIUUDPYIWGK-UHFFFAOYSA-N
Formula:	C18H36N2O2
SMILES:	CCCCCNC(=O)CCCC(=O)NCCCCC
Mol. weight [g/mol]:	312.49
CAS:	21150-82-3

Physical Properties

Property code	Value	Unit	Source
gf	21.62	kJ/mol	Joback Method
hf	-533.07	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.940		Crippen Method
mcvol	287.580	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
tb	819.32	K	Joback Method
tc	1006.77	K	Joback Method
tf	432.00 ± 1.00	K	NIST Webbook
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.81	J/mol×K	975.52	Joback Method
cpg	913.76	J/mol×K	819.32	Joback Method
cpg	930.80	J/mol×K	850.56	Joback Method
cpg	946.90	J/mol×K	881.80	Joback Method
cpg	962.07	J/mol×K	913.04	Joback Method
cpg	976.36	J/mol×K	944.28	Joback Method
cpg	1002.46	J/mol×K	1006.77	Joback Method
cps	644.70	J/mol×K	373.00	NIST Webbook
hfust	40.79	kJ/mol	432.00	NIST Webbook

hfust	4.08	kJ/mol	432.00	NIST Webbook
sfust	94.40	J/mol×K	432.00	NIST Webbook

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=C21150823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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