

Pentanamide, N,N-dinonyl-

Inchi:	InChI=1S/C23H47NO/c1-4-7-10-12-14-16-18-21-24(23(25)20-9-6-3)22-19-17-15-13-11-8
InchiKey:	IWFMNFNQQMABMT-UHFFFAOYSA-N
Formula:	C23H47NO
SMILES:	CCCCCCCCCN(CCCCCCCC)C(=O)CCCC
Mol. weight [g/mol]:	353.63

Physical Properties

Property code	Value	Unit	Source
gf	124.64	kJ/mol	Joback Method
hf	-563.10	kJ/mol	Joback Method
hfus	59.95	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.506		Crippen Method
mcvol	346.480	ml/mol	McGowan Method
pc	883.14	kPa	Joback Method
rinqol	2513.00		NIST Webbook
tb	791.95	K	Joback Method
tc	970.38	K	Joback Method
tf	431.37	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.84	J/molxK	791.95	Joback Method
cpg	1125.27	J/molxK	821.69	Joback Method
cpg	1145.63	J/molxK	851.43	Joback Method
cpg	1164.98	J/molxK	881.17	Joback Method
cpg	1183.34	J/molxK	910.91	Joback Method
cpg	1200.78	J/molxK	940.65	Joback Method
cpg	1217.32	J/molxK	970.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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