N-Methyldodecanamide

Inchi:	InChI=1S/C13H27NO/c1-3-4-5-6-7-8-9-10-11-12-13(15)14-2/h3-12H2,1-2H3,(H,14,15)
InchiKey:	APWSJINSLHHRPD-UHFFFAOYSA-N
Formula:	C13H27NO
SMILES:	CCCCCCCCCCCC(=O)NC
Mol. weight [g/mol]:	213.36
CAS:	27563-67-3

Physical Properties

Property code	Value	Unit	Source
gf	19.05	kJ/mol	Joback Method
hf	-370.76	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.653		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
tb	600.88	K	Joback Method
tc	772.66	K	Joback Method
tf	341.00 ± 3.00	K	NIST Webbook
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.48	J/mol×K	600.88	Joback Method
cpg	560.92	J/mol×K	629.51	Joback Method
cpg	576.63	J/mol×K	658.14	Joback Method
cpg	591.64	J/mol×K	686.77	Joback Method
cpg	605.98	J/mol×K	715.40	Joback Method
cpg	619.65	J/mol×K	744.03	Joback Method
cpg	632.69	J/mol×K	772.66	Joback Method
hsubt	116.60 ± 0.80	kJ/mol	330.00	NIST Webbook

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=C27563673&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
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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