

Dodecanamide, N-propyl-

Inchi:

InChI=1S/C15H31NO/c1-3-5-6-7-8-9-10-11-12-13-15(17)16-14-4-2/h3-14H2,1-2H3,(H,16)

InchiKey:

AUYWNLPGKFYZFF-UHFFFAOYSA-N

Formula:

C15H31NO

SMILES:

CCCCCCCCCCCCC(=O)NCCC

Mol. weight [g/mol]:

241.41

Physical Properties

Property code	Value	Unit	Source
gf	35.89	kJ/mol	Joback Method
hf	-412.04	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.434		Crippen Method
mcvol	233.760	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	646.64	K	Joback Method
tc	817.28	K	Joback Method
tf	361.40	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.39	J/mol×K	646.64	Joback Method
cpg	669.78	J/mol×K	675.08	Joback Method
cpg	686.40	J/mol×K	703.52	Joback Method
cpg	702.27	J/mol×K	731.96	Joback Method
cpg	717.40	J/mol×K	760.40	Joback Method
cpg	731.82	J/mol×K	788.84	Joback Method
cpg	745.57	J/mol×K	817.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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