

Propanamide, 2-methyl-N-ethyl-N-pentyl-

Inchi:	InChI=1S/C11H23NO/c1-5-7-8-9-12(6-2)11(13)10(3)4/h10H,5-9H2,1-4H3
InchiKey:	NZFLPNLTUOGOLJ-UHFFFAOYSA-N
Formula:	C11H23NO
SMILES:	CCCCCN(CC)C(=O)C(C)C
Mol. weight [g/mol]:	185.31

Physical Properties

Property code	Value	Unit	Source
gf	21.16	kJ/mol	Joback Method
hf	-320.70	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.681		Crippen Method
mvol	177.400	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	516.95	K	Joback Method
tc	690.14	K	Joback Method
tf	281.13	K	Joback Method
vc	0.669	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.60	J/mol×K	516.95	Joback Method
cpg	439.82	J/mol×K	545.82	Joback Method
cpg	455.32	J/mol×K	574.68	Joback Method
cpg	470.13	J/mol×K	603.55	Joback Method
cpg	484.26	J/mol×K	632.41	Joback Method
cpg	497.74	J/mol×K	661.28	Joback Method
cpg	510.58	J/mol×K	690.14	Joback Method

Sources

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=U415343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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