

Acetamide, N-butyl-N-pentyl-

Inchi:	InChI=1S/C11H23NO/c1-4-6-8-10-12(11(3)13)9-7-5-2/h4-10H2,1-3H3
InchiKey:	LDFFOFNDFZWNCU-UHFFFAOYSA-N
Formula:	C11H23NO
SMILES:	CCCCCN(CCCC)C(C)=O
Mol. weight [g/mol]:	185.31

Physical Properties

Property code	Value	Unit	Source
gf	23.60	kJ/mol	Joback Method
hf	-315.42	kJ/mol	Joback Method
hfus	28.87	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.825		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
tb	517.39	K	Joback Method
tc	687.29	K	Joback Method
tf	296.13	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.40	J/mol×K	517.39	Joback Method
cpg	439.24	J/mol×K	545.71	Joback Method
cpg	454.41	J/mol×K	574.02	Joback Method
cpg	468.91	J/mol×K	602.34	Joback Method
cpg	482.76	J/mol×K	630.66	Joback Method
cpg	496.00	J/mol×K	658.97	Joback Method
cpg	508.63	J/mol×K	687.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415741&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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