

Acetamide, N-butyl-N-nonyl-

Inchi:	InChI=1S/C15H31NO/c1-4-6-8-9-10-11-12-14-16(15(3)17)13-7-5-2/h4-14H2,1-3H3
InchiKey:	MBCJPASARJPKAY-UHFFFAOYSA-N
Formula:	C15H31NO
SMILES:	CCCCCCCCCN(CCCC)C(C)=O
Mol. weight [g/mol]:	241.41

Physical Properties

Property code	Value	Unit	Source
gf	57.28	kJ/mol	Joback Method
hf	-397.98	kJ/mol	Joback Method
hfus	39.23	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.386		Crippen Method
mcvol	233.760	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
tb	608.91	K	Joback Method
tc	775.35	K	Joback Method
tf	341.21	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.00	J/molxK	608.91	Joback Method
cpg	647.99	J/molxK	636.65	Joback Method
cpg	665.20	J/molxK	664.39	Joback Method
cpg	681.65	J/molxK	692.13	Joback Method
cpg	697.35	J/molxK	719.87	Joback Method
cpg	712.34	J/molxK	747.61	Joback Method
cpg	726.65	J/molxK	775.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415747&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
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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