Acetamide, N-butyl-N-propyl-

Inchi: InChI=1S/C9H19NO/c1-4-6-8-10(7-5-2)9(3)11/h4-8H2,1-3H3
InchiKey: XOKMSKQWQKSTDN-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCCN(CCC)C(C)=O
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
gf	6.76	kJ/mol	Joback Method
hf	-274.14	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.045		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	471.63	K	Joback Method
tc	644.09	K	Joback Method
tf	273.59	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.21	J/mol×K	471.63	Joback Method
cpg	344.54	J/mol×K	500.37	Joback Method
cpg	358.27	J/mol×K	529.12	Joback Method
cpg	371.39	J/mol×K	557.86	Joback Method
cpg	383.93	J/mol×K	586.60	Joback Method
cpg	395.91	J/mol×K	615.35	Joback Method
cpg	407.34	J/mol×K	644.09	Joback Method

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=U415737&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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