Acetamide, N-butyl-

Other names: N-Butylacetamide
N-n-Butylacetamide
Inchi: InChI=1S/C6H13NO/c1-3-4-5-7-6(2)8/h3-5H2,1-2H3,(H,7,8)
InchiKey: GYLDXXLJMRTVSS-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CCCCNC(C)=O
Mol. weight [g/mol]: 115.17
CAS: 1119-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-39.89	kJ/mol	Joback Method
hf	-226.28	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	75.00 ± 0.30	kJ/mol	NIST Webbook
hvap	76.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.30		Crippen Method
logp	0.923		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
ripol	1885.00		NIST Webbook
tb	502.20	K	NIST Webbook
tc	622.63	K	Joback Method
tf	259.97	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.42	J/mol×K	440.72	Joback Method
cpg	229.26	J/mol×K	471.04	Joback Method

cpg	239.64	J/mol×K	501.36	Joback Method
cpg	249.58	J/mol×K	531.67	Joback Method
cpg	259.09	J/mol×K	561.99	Joback Method
cpg	268.18	J/mol×K	592.31	Joback Method
cpg	276.87	J/mol×K	622.63	Joback Method
cpl	236.89	J/mol×K	298.15	NIST Webbook
cpl	236.00	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55638e+01
Coeff. B	-4.61298e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	382.72
Temperature range (K), max.	530.69

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=C1119499&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

cpl: Liquid phase 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume