Acetanilide, n-butyl-

Other names: N-butylacetanilide
Acetamide, N-butyl-N-phenyl-
Inchi: InChI=1S/C12H17NO/c1-3-4-10-13(11(2)14)12-8-6-5-7-9-12/h5-9H,3-4,10H2,1-2H3
InchiKey: ZWDZJRRQSXLOQR-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCCCN(C(C)=O)c1ccccc1
Mol. weight [g/mol]: 191.27
CAS: 91-49-6

Physical Properties

Property code	Value	Unit	Source
gf	144.43	kJ/mol	Joback Method
hf	-99.53	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.840		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	554.20	K	NIST Webbook
tc	772.19	K	Joback Method
tf	297.60 ± 0.02	K	NIST Webbook
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.27	J/mol×K	737.99	Joback Method
cpg	404.29	J/mol×K	566.95	Joback Method
cpg	420.36	J/mol×K	601.16	Joback Method
cpg	435.45	J/mol×K	635.36	Joback Method
cpg	449.60	J/mol×K	669.57	Joback Method
cpg	462.86	J/mol×K	703.78	Joback Method
cpg	486.87	J/mol×K	772.19	Joback Method

hvapt	60.20	kJ/mol	548.00	NIST Webbook

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=C91496&Units=SI
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
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume