acetamide, N-butyl-N-phenyl-

Other names: Acetamide, N-butyl-N-phenyl-
N-butylacetanilide
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

Physical Properties

Property code	Value	Unit	Source
hfus	25.50	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	2.840		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
tb	554.20	K	NIST Webbook
tf	297.60 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	475.27	J/mol×K	737.99	Joback Method
cpg	486.87	J/mol×K	772.19	Joback Method
hvapt	60.20	kJ/mol	548.00	NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91496&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point