Acetamide, 2-phenyl-N-butyl-N-ethyl-

Inchi: InChI=1S/C14H21NO/c1-3-5-11-15(4-2)14(16)12-13-9-7-6-8-10-13/h6-10H,3-5,11-12H2,
InchiKey: UVWHMIMTPOWHCH-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCN(CC)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
gf	161.27	kJ/mol	Joback Method
hf	-140.81	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.878		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
tb	612.71	K	Joback Method
tc	812.07	K	Joback Method
tf	356.36	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.79	J/mol×K	612.71	Joback Method
cpg	521.85	J/mol×K	645.94	Joback Method
cpg	537.90	J/mol×K	679.16	Joback Method
cpg	552.98	J/mol×K	712.39	Joback Method
cpg	567.15	J/mol×K	745.62	Joback Method
cpg	580.45	J/mol×K	778.84	Joback Method
cpg	592.92	J/mol×K	812.07	Joback Method

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=U415668&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
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