Acetamide, 2-phenyl-N-butyl-N-isobutyl-

Inchi: InChI=1S/C16H25NO/c1-4-5-11-17(13-14(2)3)16(18)12-15-9-7-6-8-10-15/h6-10,14H,4-5
InchiKey: MDCSFNVSHFYXME-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCN(CC(C)C)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	175.67	kJ/mol	Joback Method
hf	-187.37	kJ/mol	Joback Method
hfus	32.33	kJ/mol	Joback Method
hvap	61.89	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.514		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	658.03	K	Joback Method
tc	855.92	K	Joback Method
tf	363.90	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.37	J/mol×K	658.03	Joback Method
cpg	629.48	J/mol×K	691.01	Joback Method
cpg	646.51	J/mol×K	723.99	Joback Method
cpg	662.53	J/mol×K	756.97	Joback Method
cpg	677.57	J/mol×K	789.95	Joback Method
cpg	691.69	J/mol×K	822.94	Joback Method
cpg	704.94	J/mol×K	855.92	Joback Method

Sources

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=U415670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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