Acetamide, 2-phenyl-N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C17H27NO/c1-4-5-12-18(13-11-15(2)3)17(19)14-16-9-7-6-8-10-16/h6-10,15H,
InchiKey: ZBVGZBCISIESDP-UHFFFAOYSA-N
Formula: C17H27NO
SMILES: CCCCN(CCC(C)C)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 261.40

Physical Properties

Property code	Value	Unit	Source
gf	184.09	kJ/mol	Joback Method
hf	-208.01	kJ/mol	Joback Method
hfus	34.92	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	680.91	K	Joback Method
tc	876.64	K	Joback Method
tf	375.17	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.36	J/mol×K	680.91	Joback Method
cpg	684.73	J/mol×K	713.53	Joback Method
cpg	702.02	J/mol×K	746.15	Joback Method
cpg	718.28	J/mol×K	778.78	Joback Method
cpg	733.57	J/mol×K	811.40	Joback Method
cpg	747.93	J/mol×K	844.02	Joback Method
cpg	761.43	J/mol×K	876.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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