

Acetamide, 2-phenyl-N-butyl-N-pentyl-

Inchi:	InChI=1S/C17H27NO/c1-3-5-10-14-18(13-6-4-2)17(19)15-16-11-8-7-9-12-16/h7-9,11-12
InchiKey:	IQBAVUVYGSVLKI-UHFFFAOYSA-N
Formula:	C17H27NO
SMILES:	CCCCCN(CCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]:	261.40

Physical Properties

Property code	Value	Unit	Source
gf	186.53	kJ/mol	Joback Method
hf	-202.73	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mvol	238.180	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	681.35	K	Joback Method
tc	873.98	K	Joback Method
tf	390.17	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.91	J/mol×K	681.35	Joback Method
cpg	683.95	J/mol×K	713.45	Joback Method
cpg	700.96	J/mol×K	745.56	Joback Method
cpg	716.99	J/mol×K	777.66	Joback Method
cpg	732.08	J/mol×K	809.77	Joback Method
cpg	746.28	J/mol×K	841.87	Joback Method
cpg	759.64	J/mol×K	873.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415673&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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