

Acetamide, 2-phenyl-N-butyl-N-propyl-

Inchi:	InChI=1S/C15H23NO/c1-3-5-12-16(11-4-2)15(17)13-14-9-7-6-8-10-14/h6-10H,3-5,11-13
InchiKey:	KYRKFRQVNZBOKJ-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCN(CCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]:	233.35

Physical Properties

Property code	Value	Unit	Source
gf	169.69	kJ/mol	Joback Method
hf	-161.45	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.268		Crippen Method
mvol	210.000	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	635.59	K	Joback Method
tc	832.38	K	Joback Method
tf	367.63	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.20	J/mol×K	635.59	Joback Method
cpg	574.64	J/mol×K	668.39	Joback Method
cpg	591.06	J/mol×K	701.19	Joback Method
cpg	606.51	J/mol×K	733.98	Joback Method
cpg	621.04	J/mol×K	766.78	Joback Method
cpg	634.68	J/mol×K	799.58	Joback Method
cpg	647.49	J/mol×K	832.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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