Acetamide, 2-phenyl-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C19H31NO/c1-4-6-9-12-17(3)20(15-7-5-2)19(21)16-18-13-10-8-11-14-18/h8,10
InchiKey: JLMXKLARNZPTNZ-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CCCCCC(C)N(CCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	200.93	kJ/mol	Joback Method
hf	-249.29	kJ/mol	Joback Method
hfus	40.10	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.827		Crippen Method
mcvol	266.360	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
tb	726.67	K	Joback Method
tc	919.33	K	Joback Method
tf	397.71	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.75	J/mol×K	726.67	Joback Method
cpg	798.54	J/mol×K	758.78	Joback Method
cpg	816.24	J/mol×K	790.89	Joback Method
cpg	832.91	J/mol×K	823.00	Joback Method
cpg	848.60	J/mol×K	855.11	Joback Method
cpg	863.36	J/mol×K	887.22	Joback Method
cpg	877.24	J/mol×K	919.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415674&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
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