Propanamide, 3-phenyl-N-propyl-

Inchi: InChI=1S/C12H17NO/c1-2-10-13-12(14)9-8-11-6-4-3-5-7-11/h3-7H,2,8-10H2,1H3,(H,13,
InchiKey: IYWLQMRIMWEQQC-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCCNC(=O)CCc1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	123.04	kJ/mol	Joback Method
hf	-113.59	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.145		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	604.68	K	Joback Method
tc	812.84	K	Joback Method
tf	354.01	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.04	J/mol×K	604.68	Joback Method
cpg	435.26	J/mol×K	639.37	Joback Method
cpg	449.55	J/mol×K	674.07	Joback Method
cpg	462.95	J/mol×K	708.76	Joback Method
cpg	475.50	J/mol×K	743.46	Joback Method
cpg	487.24	J/mol×K	778.15	Joback Method
cpg	498.21	J/mol×K	812.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407148&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