Pentanamide, N-phenyl-

Other names: Valeranilide
Inchi: InChI=1S/C11H15NO/c1-2-3-9-11(13)12-10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3,(H,12,13)
InchiKey: PGMBORLSOHYBFJ-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCCCC(=O)Nc1ccccc1
Mol. weight [g/mol]: 177.24
CAS: 10264-18-3

Physical Properties

Property code	Value	Unit	Source
gf	114.62	kJ/mol	Joback Method
hf	-92.95	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	55.54	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.815		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	581.80	K	Joback Method
tc	793.35	K	Joback Method
tf	342.74	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.18	J/mol×K	581.80	Joback Method
cpg	385.78	J/mol×K	617.06	Joback Method
cpg	399.48	J/mol×K	652.32	Joback Method
cpg	412.31	J/mol×K	687.58	Joback Method
cpg	424.31	J/mol×K	722.84	Joback Method
cpg	435.52	J/mol×K	758.09	Joback Method

cpg	445.98	J/mol×K	793.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10264183&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