Propanamide, 2,2-dimethyl-N-phenyl-

Other names: Pivalanilide
Inchi: InChI=1S/C11H15NO/c1-11(2,3)10(13)12-9-7-5-4-6-8-9/h4-8H,1-3H3,(H,12,13)
InchiKey: LWJNWXYSLBGWDU-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CC(C)(C)C(=O)Nc1ccccc1
Mol. weight [g/mol]: 177.24
CAS: 6625-74-7

Physical Properties

Property code	Value	Unit	Source
gf	117.46	kJ/mol	Joback Method
hf	-101.70	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	54.24	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.671		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1465.00		NIST Webbook
tb	578.57	K	Joback Method
tc	803.27	K	Joback Method
tf	345.16	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.54	J/mol×K	578.57	Joback Method
cpg	390.02	J/mol×K	616.02	Joback Method
cpg	404.37	J/mol×K	653.47	Joback Method
cpg	417.65	J/mol×K	690.92	Joback Method
cpg	429.94	J/mol×K	728.37	Joback Method
cpg	441.31	J/mol×K	765.82	Joback Method
cpg	451.81	J/mol×K	803.27	Joback Method

Sources

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=C6625747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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