

Butanamide, N-phenyl-

Other names:	n-Butyranilide Butyranilide Butyrylanilide N-Phenylbutyramide
Inchi:	InChI=1S/C10H13NO/c1-2-6-10(12)11-9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3,(H,11,12)
InchiKey:	UHANVDZCDNSILX-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CCCC(=O)Nc1ccccc1
Mol. weight [g/mol]:	163.22
CAS:	1129-50-6

Physical Properties

Property code	Value	Unit	Source
gf	106.20	kJ/mol	Joback Method
hf	-72.31	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.425		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	558.92	K	Joback Method
tc	774.06	K	Joback Method
tf	331.47	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.93	J/mol×K	558.92	Joback Method
cpg	337.81	J/mol×K	594.78	Joback Method
cpg	350.81	J/mol×K	630.63	Joback Method

cpg	362.97	J/mol×K	666.49	Joback Method
cpg	374.33	J/mol×K	702.34	Joback Method
cpg	384.93	J/mol×K	738.20	Joback Method
cpg	394.80	J/mol×K	774.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1129506&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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