

isobutyranilide

Other names:	Isobutyric acid anilide Propanamide, 2-methyl-N-phenyl- i-Butyranilide
Inchi:	InChI=1S/C10H13NO/c1-8(2)10(12)11-9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)
InchiKey:	WDRCPKDLZOQCFU-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CC(C)C(=O)Nc1ccccc1
Mol. weight [g/mol]:	163.22
CAS:	4406-41-1

Physical Properties

Property code	Value	Unit	Source
gf	103.76	kJ/mol	Joback Method
hf	-77.59	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.281		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1484.00		NIST Webbook
tb	558.48	K	Joback Method
tc	778.35	K	Joback Method
tf	316.47	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	558.48	Joback Method
cpg	338.54	J/mol×K	595.12	Joback Method
cpg	351.86	J/mol×K	631.77	Joback Method
cpg	364.30	J/mol×K	668.41	Joback Method
cpg	375.89	J/mol×K	705.06	Joback Method

cpg	386.67	J/mol×K	741.70	Joback Method
cpg	396.68	J/mol×K	778.35	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=C4406411&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

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