

Benzamide, N-isobutyl-

Inchi:	InChI=1S/C11H15NO/c1-9(2)8-12-11(13)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3,(H,12,13)
InchiKey:	ZABMXPJUCKVZSH-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CC(C)CNC(=O)c1ccccc1
Mol. weight [g/mol]:	177.24
CAS:	5705-57-7

Physical Properties

Property code	Value	Unit	Source
gf	112.18	kJ/mol	Joback Method
hf	-98.23	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.072		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1560.00		NIST Webbook
tb	581.36	K	Joback Method
tc	797.40	K	Joback Method
tf	327.74	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.57	J/mol×K	581.36	Joback Method
cpg	386.54	J/mol×K	617.37	Joback Method
cpg	400.55	J/mol×K	653.37	Joback Method
cpg	413.65	J/mol×K	689.38	Joback Method
cpg	425.88	J/mol×K	725.38	Joback Method
cpg	437.28	J/mol×K	761.39	Joback Method
cpg	447.88	J/mol×K	797.40	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=C5705577&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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