

Benzamide, N-(1,1-dimethylethyl)-N-methyl-

Other names:	N-(1,1-dimethylethyl)-N-methyl-benzamide
Inchi:	InChI=1S/C12H17NO/c1-12(2,3)13(4)11(14)10-8-6-5-7-9-10/h5-9H,1-4H3
InchiKey:	IWHZLXOVOHSRPU-UHFFFAOYSA-N
Formula:	C12H17NO
SMILES:	CN(C(=O)c1ccccc1)C(C)(C)C
Mol. weight [g/mol]:	191.27
CAS:	49690-12-2

Physical Properties

Property code	Value	Unit	Source
gf	147.27	kJ/mol	Joback Method
hf	-108.28	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.557		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1514.54		NIST Webbook
rinpol	1502.73		NIST Webbook
rinpol	1547.20		NIST Webbook
rinpol	1502.73		NIST Webbook
rinpol	1535.11		NIST Webbook
ripol	2365.65		NIST Webbook
ripol	2377.69		NIST Webbook
ripol	2389.32		NIST Webbook
ripol	2365.65		NIST Webbook
tb	563.72	K	Joback Method
tc	781.64	K	Joback Method
tf	336.24	K	Joback Method
vc	0.613	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.47	J/mol×K	563.72	Joback Method
cpg	424.56	J/mol×K	600.04	Joback Method
cpg	440.44	J/mol×K	636.36	Joback Method
cpg	455.16	J/mol×K	672.68	Joback Method
cpg	468.82	J/mol×K	709.00	Joback Method
cpg	481.47	J/mol×K	745.32	Joback Method
cpg	493.20	J/mol×K	781.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49690122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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