N-(2,2-dimethylpropyl)-N-methyl-benzamide

Inchi: InChI=1S/C13H19NO/c1-13(2,3)10-14(4)12(15)11-8-6-5-7-9-11/h5-9H,10H2,1-4H3
InchiKey: NXLPXQWESLPQSU-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CN(CC(C)(C)C)C(=O)c1ccccc1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
gf	155.69	kJ/mol	Joback Method
hf	-128.92	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	54.30	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.805		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1637.79		NIST Webbook
rinpol	1606.54		NIST Webbook
rinpol	1657.39		NIST Webbook
rinpol	1625.88		NIST Webbook
rinpol	1606.54		NIST Webbook
ripol	2472.23		NIST Webbook
ripol	2510.89		NIST Webbook
ripol	2491.77		NIST Webbook
ripol	2472.23		NIST Webbook
tb	586.60	K	Joback Method
tc	800.78	K	Joback Method
tf	347.51	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.88	J/mol×K	586.60	Joback Method

cpg	474.44	J/mol×K	622.30	Joback Method
cpg	490.78	J/mol×K	657.99	Joback Method
cpg	505.97	J/mol×K	693.69	Joback Method
cpg	520.10	J/mol×K	729.39	Joback Method
cpg	533.23	J/mol×K	765.09	Joback Method
cpg	545.43	J/mol×K	800.78	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=R194037&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume