Benzamide, 4-methyl-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H19NO/c1-10(2)8-9-14-13(15)12-6-4-11(3)5-7-12/h4-7,10H,8-9H2,1-3H3,(
InchiKey: AVLHVSHTWPMHEE-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: Cc1ccc(C(=O)NCCC(C)C)cc1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
gf	119.39	kJ/mol	Joback Method
hf	-150.98	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.771		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook
tb	632.10	K	Joback Method
tc	842.01	K	Joback Method
tf	362.80	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.41	J/mol×K	632.10	Joback Method
cpg	486.29	J/mol×K	667.08	Joback Method
cpg	501.21	J/mol×K	702.07	Joback Method
cpg	515.22	J/mol×K	737.05	Joback Method
cpg	528.35	J/mol×K	772.04	Joback Method
cpg	540.63	J/mol×K	807.02	Joback Method
cpg	552.10	J/mol×K	842.01	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=U407467&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