N-(1-methylpropyl)-N-methyl-benzamide

Inchi: InChI=1S/C12H17NO/c1-4-10(2)13(3)12(14)11-8-6-5-7-9-11/h5-10H,4H2,1-3H3
InchiKey: BRCXRESFUXLPOM-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCC(C)N(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	141.99	kJ/mol	Joback Method
hf	-104.81	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.557		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1603.84		NIST Webbook
rinpol	1617.16		NIST Webbook
rinpol	1634.08		NIST Webbook
rinpol	1580.72		NIST Webbook
rinpol	1582.36		NIST Webbook
rinpol	1567.69		NIST Webbook
rinpol	1594.83		NIST Webbook
rinpol	1621.60		NIST Webbook
ripol	2475.52		NIST Webbook
ripol	2463.28		NIST Webbook
ripol	2447.50		NIST Webbook
ripol	2460.44		NIST Webbook
ripol	2434.25		NIST Webbook
ripol	2450.89		NIST Webbook
tb	566.51	K	Joback Method
tc	776.09	K	Joback Method
tf	318.82	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.63	J/mol×K	566.51	Joback Method
cpg	421.10	J/mol×K	601.44	Joback Method
cpg	436.54	J/mol×K	636.37	Joback Method
cpg	450.99	J/mol×K	671.30	Joback Method
cpg	464.50	J/mol×K	706.23	Joback Method
cpg	477.12	J/mol×K	741.16	Joback Method
cpg	488.90	J/mol×K	776.09	Joback Method

Sources

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=R194002&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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