N-Butyl-N-methyl-benzamide

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

Physical Properties

Property code	Value	Unit	Source
gf	144.43	kJ/mol	Joback Method
hf	-99.53	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.559		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1621.37		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1664.78		NIST Webbook
rinpol	1644.21		NIST Webbook
rinpol	1641.72		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1621.37		NIST Webbook
ripol	2554.04		NIST Webbook
ripol	2594.85		NIST Webbook
ripol	2554.04		NIST Webbook
ripol	2574.33		NIST Webbook
tb	566.95	K	Joback Method
tc	772.19	K	Joback Method
tf	333.82	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.29	J/mol×K	566.95	Joback Method
cpg	420.36	J/mol×K	601.16	Joback Method
cpg	435.45	J/mol×K	635.36	Joback Method
cpg	449.60	J/mol×K	669.57	Joback Method
cpg	462.86	J/mol×K	703.78	Joback Method
cpg	475.27	J/mol×K	737.99	Joback Method
cpg	486.87	J/mol×K	772.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R194062&Units=SI
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

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