Benzamide, 4-methyl-N-butyl-

Inchi: InChI=1S/C12H17NO/c1-3-4-9-13-12(14)11-7-5-10(2)6-8-11/h5-8H,3-4,9H2,1-2H3,(H,13
InchiKey: VYVZZAYSPZXQDQ-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCCCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	113.41	kJ/mol	Joback Method
hf	-125.06	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.525		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1785.00		NIST Webbook
tb	609.66	K	Joback Method
tc	818.77	K	Joback Method
tf	366.53	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.59	J/mol×K	609.66	Joback Method
cpg	434.57	J/mol×K	644.51	Joback Method
cpg	448.67	J/mol×K	679.36	Joback Method
cpg	461.92	J/mol×K	714.21	Joback Method
cpg	474.35	J/mol×K	749.07	Joback Method
cpg	485.99	J/mol×K	783.92	Joback Method
cpg	496.89	J/mol×K	818.77	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=U407466&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