

Benzamide, 4-methyl-N-(4-methylbenzoyl)-N-butyl-

Inchi:	InChI=1S/C20H23NO2/c1-4-5-14-21(19(22)17-10-6-15(2)7-11-17)20(23)18-12-8-16(3)9-
InchiKey:	BXXJZMAPIZJYMA-UHFFFAOYSA-N
Formula:	C20H23NO2
SMILES:	CCCCN(C(=O)c1ccc(C)cc1)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	309.40

Physical Properties

Property code	Value	Unit	Source
gf	176.02	kJ/mol	Joback Method
hf	-163.64	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.386		Crippen Method
mvol	258.260	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	840.50	K	Joback Method
tc	1065.75	K	Joback Method
tf	525.37	K	Joback Method
vc	0.970	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.71	J/mol×K	840.50	Joback Method
cpg	782.02	J/mol×K	878.04	Joback Method
cpg	796.16	J/mol×K	915.58	Joback Method
cpg	809.21	J/mol×K	953.12	Joback Method
cpg	821.24	J/mol×K	990.66	Joback Method
cpg	832.33	J/mol×K	1028.21	Joback Method
cpg	842.57	J/mol×K	1065.75	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=U407482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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