

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

Inchi:	InChI=1S/C21H25NO2/c1-4-5-6-15-22(20(23)18-11-7-16(2)8-12-18)21(24)19-13-9-17(3)
InchiKey:	GOCISPBLEOEVGR-UHFFFAOYSA-N
Formula:	C21H25NO2
SMILES:	CCCCCN(C(=O)c1ccc(C)cc1)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	323.43

Physical Properties

Property code	Value	Unit	Source
gf	184.44	kJ/mol	Joback Method
hf	-184.28	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	83.75	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.776		Crippen Method
mvol	272.350	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	863.38	K	Joback Method
tc	1086.51	K	Joback Method
tf	536.64	K	Joback Method
vc	1.026	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.40	J/mol×K	863.38	Joback Method
cpg	839.86	J/mol×K	900.57	Joback Method
cpg	854.15	J/mol×K	937.76	Joback Method
cpg	867.35	J/mol×K	974.95	Joback Method
cpg	879.55	J/mol×K	1012.13	Joback Method
cpg	890.82	J/mol×K	1049.32	Joback Method
cpg	901.24	J/mol×K	1086.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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