Benzamide, 4-methyl-N-(4-methylbenzoyl)-N-(3-methylbutyl)-

Inchi: InChI=1S/C21H25NO2/c1-15(2)13-14-22(20(23)18-9-5-16(3)6-10-18)21(24)19-11-7-17(4

InchiKey: UMNWNGXHXNEDPR-UHFFFAOYSA-N

Formula: C21H25NO2

SMILES: Cc1ccc(C(=O)N(CCC(C)C)C(=O)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 323.43

Physical Properties

Property code	Value	Unit	Source
gf	182.00	kJ/mol	Joback Method
hf	-189.56	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.632		Crippen Method
mcvol	272.350	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	862.94	K	Joback Method
tc	1089.01	K	Joback Method
tf	521.64	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.94	J/mol×K	862.94	Joback Method
cpg	840.57	J/mol×K	900.62	Joback Method
cpg	854.99	J/mol×K	938.30	Joback Method
cpg	868.29	J/mol×K	975.97	Joback Method
cpg	880.54	J/mol×K	1013.65	Joback Method
cpg	891.82	J/mol×K	1051.33	Joback Method
cpg	902.24	J/mol×K	1089.01	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=U407483&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume