Benzoic acid, 4-di(3-methylbutyl)amino-, methyl ester

Inchi: InChI=1S/C18H29NO2/c1-14(2)10-12-19(13-11-15(3)4)17-8-6-16(7-9-17)18(20)21-5/h6-9

InchiKey: OJCZKWKMSHWFPE-UHFFFAOYSA-N

Formula: C18H29NO2

SMILES: COC(=O)c1ccc(N(CCC(C)C)CCC(C)C)cc1

Mol. weight [g/mol]: 291.43

Physical Properties

Property code	Value	Unit	Source
gf	75.44	kJ/mol	Joback Method
hf	-377.62	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.372		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	730.75	K	Joback Method
tc	927.66	K	Joback Method
tf	406.19	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.95	J/mol×K	730.75	Joback Method
cpg	771.23	J/mol×K	763.57	Joback Method
cpg	788.42	J/mol×K	796.39	Joback Method
cpg	804.56	J/mol×K	829.20	Joback Method
cpg	819.68	J/mol×K	862.02	Joback Method
cpg	833.83	J/mol×K	894.84	Joback Method
cpg	847.04	J/mol×K	927.66	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=U375353&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