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

Inchi: InChI=1S/C22H37NO2/c1-17(2)10-13-23(14-11-18(3)4)21-9-7-8-20(16-21)22(24)25-15-1

InchiKey: JUEMSBZDBDVDFO-UHFFFAOYSA-N

Formula: C22H37NO2

SMILES: CC(C)CCOC(=O)c1cccc(N(CCC(C)C)CCC(C)C)c1

Mol. weight [g/mol]: 347.53

Physical Properties

Property code	Value	Unit	Source
gf	106.68	kJ/mol	Joback Method
hf	-465.46	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.788		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	821.83	K	Joback Method
tc	1019.18	K	Joback Method
tf	436.27	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.88	J/mol×K	821.83	Joback Method
cpg	1009.04	J/mol×K	854.72	Joback Method
cpg	1027.01	J/mol×K	887.61	Joback Method
cpg	1043.81	J/mol×K	920.51	Joback Method
cpg	1059.50	J/mol×K	953.40	Joback Method
cpg	1074.13	J/mol×K	986.29	Joback Method
cpg	1087.75	J/mol×K	1019.18	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=U375449&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