Benzoic acid, p-(dimethylamino-), isopentyl ester

Other names: padimate
Inchi: InChI=1S/C14H21NO2/c1-11(2)9-10-17-14(16)12-5-7-13(8-6-12)15(3)4/h5-8,11H,9-10H2
InchiKey: OFSAUHSCHWRZKM-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CC(C)CCOC(=O)c1ccc(N(C)C)cc1
Mol. weight [g/mol]: 235.32
CAS: 21245-01-2

Physical Properties

Property code	Value	Unit	Source
gf	44.20	kJ/mol	Joback Method
hf	-289.78	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.955		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	639.67	K	Joback Method
tc	841.91	K	Joback Method
tf	376.11	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.69	J/mol×K	639.67	Joback Method
cpg	549.46	J/mol×K	673.38	Joback Method
cpg	565.26	J/mol×K	707.08	Joback Method
cpg	580.12	J/mol×K	740.79	Joback Method
cpg	594.06	J/mol×K	774.50	Joback Method
cpg	607.13	J/mol×K	808.21	Joback Method
cpg	619.34	J/mol×K	841.91	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=C21245012&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume