Benzyl 2,2-diphenyl-3-dimethylamino propionate

Inchi: InChI=1S/C24H25NO2/c1-25(2)19-24(21-14-8-4-9-15-21,22-16-10-5-11-17-22)23(26)27-

InchiKey: IWBYIIHCUJCVRE-UHFFFAOYSA-N

Formula: C24H25NO2

SMILES: CN(C)CC(C(=O)OCc1ccccc1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 359.46

CAS: 116594-69-5

Physical Properties

Property code	Value	Unit	Source
gf	368.13	kJ/mol	Joback Method
hf	-15.12	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.278		Crippen Method
mcvol	295.160	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
tb	914.06	K	Joback Method
tc	1161.22	K	Joback Method
tf	546.55	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.43	J/mol×K	914.06	Joback Method
cpg	933.27	J/mol×K	955.25	Joback Method
cpg	947.76	J/mol×K	996.45	Joback Method
cpg	961.08	J/mol×K	1037.64	Joback Method
cpg	973.40	J/mol×K	1078.83	Joback Method
cpg	984.88	J/mol×K	1120.03	Joback Method
cpg	995.68	J/mol×K	1161.22	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=C116594695&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume