2-Butanol, 4-dimethylamino-3-methyl-1,2-diphenyl-, propionate

Inchi: InChI=1S/C22H29NO2/c1-5-21(24)25-22(18(2)17-23(3)4,20-14-10-7-11-15-20)16-19-12-
InchiKey: XLMALTXPSGQGBX-UHFFFAOYSA-N
Formula: C22H29NO2
SMILES: CCC(=O)OC(Cc1ccccc1)(c1ccccc1)C(C)CN(C)C
Mol. weight [g/mol]: 339.47
CAS: 77-50-9

Physical Properties

Property code	Value	Unit	Source
gf	236.44	kJ/mol	Joback Method
hf	-215.65	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.276		Crippen Method
mcvol	290.740	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
tb	841.18	K	Joback Method
tc	1064.91	K	Joback Method
tf	482.59	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.37	J/mol×K	841.18	Joback Method
cpg	916.02	J/mol×K	878.47	Joback Method
cpg	932.33	J/mol×K	915.76	Joback Method
cpg	947.42	J/mol×K	953.04	Joback Method
cpg	961.38	J/mol×K	990.33	Joback Method
cpg	974.34	J/mol×K	1027.62	Joback Method
cpg	986.39	J/mol×K	1064.91	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=C77509&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