2(3H)-Benzofuranone, 3-(«beta»-diethylaminoethyl)-3-phenyl-

Other names: Amethone
Amocaine
Amolanone
AP 43
Butyric acid, 4-(diethylamino)-2-(o-hydroxyphenyl)-2-phenyl-, «gamma»-lactone
3-(«beta»-Diethylaminoethyl)-3-phenyl-2-benzofuranone
3-(«beta»-Diethylaminoethyl)-3-phenyl-2-(3H)-benzofuranone
3-(2-(Diethylamino)ethyl)-3-phenyl-2(3H)-benzofuranone
«gamma»-Diethylamino-«alpha»-(o-hydroxyphenyl)-«alpha»-phenylbutyric acid lactone
3-(2-(Diethylamino)ethyl)-2-oxo-3-phenyl-2,3-dihydrobenzofuran
2(3H)-Benzofuranone, 3-[2-(diethylamino)ethyl]-3-phenyl-
Amethone base

Inchi: InChI=1S/C20H23NO2/c1-3-21(4-2)15-14-20(16-10-6-5-7-11-16)17-12-8-9-13-18(17)23-
InchiKey: HPITVGRITATAFY-UHFFFAOYSA-N
Formula: C20H23NO2
SMILES: CCN(CC)CCC1(c2ccccc2)C(=O)Oc2ccccc21
Mol. weight [g/mol]: 309.40
CAS: 76-65-3

Physical Properties

Property code	Value	Unit	Source
gf	290.04	kJ/mol	Joback Method
hf	-108.67	kJ/mol	Joback Method
hfus	37.60	kJ/mol	Joback Method
hvap	74.89	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.624		Crippen Method
mcvol	251.700	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2226.00		NIST Webbook
tb	829.53	K	Joback Method
tc	1069.37	K	Joback Method
tf	549.62	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.94	J/mol×K	829.53	Joback Method
cpg	795.93	J/mol×K	869.50	Joback Method
cpg	814.31	J/mol×K	909.48	Joback Method
cpg	832.29	J/mol×K	949.45	Joback Method
cpg	850.09	J/mol×K	989.42	Joback Method
cpg	867.94	J/mol×K	1029.40	Joback Method
cpg	886.05	J/mol×K	1069.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76653&Units=SI
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

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