Benzeneacetic acid, «alpha»-phenyl-, 2-(diethylamino)ethyl ester

Other names: Acetic acid, diphenyl-, 2-(diethylamino)ethyl ester
Adiphenin
Adiphenine
2-Diethylaminoethyl diphenylacetate
2-Diethylaminoethylester kyseliny difenyloctove
Difacil
Diphacil
Diphacyl
Diphenylacetic acid diethylaminoethyl ester
Diphenylacetic acid, 2-(diethylamino)ethyl ester
Diphenylacetyldiethylaminoethanol
Patrovine
Spasmolytin
Transentine
Tranzetil
Trasentin
Trasentine
Trazentyna
Vegantine
Wegantyna
SKF 962A

Inchi: InChI=1S/C20H25NO2/c1-3-21(4-2)15-16-23-20(22)19(17-11-7-5-8-12-17)18-13-9-6-10-

InchiKey: JGOAIQNSOGZNBX-UHFFFAOYSA-N

Formula: C20H25NO2

SMILES: CCN(CC)CCOC(=O)C(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 311.42

CAS: 64-95-9

Physical Properties

Property code	Value	Unit	Source
gf	216.76	kJ/mol	Joback Method
hf	-165.62	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.704		Crippen Method

mcvol	262.560	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2186.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2192.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	798.65	K	Joback Method
tc	1018.16	K	Joback Method
tf	457.63	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.75	J/mol×K	798.65	Joback Method
cpg	797.91	J/mol×K	835.23	Joback Method
cpg	813.77	J/mol×K	871.82	Joback Method
cpg	828.41	J/mol×K	908.40	Joback Method
cpg	841.90	J/mol×K	944.99	Joback Method
cpg	854.31	J/mol×K	981.57	Joback Method
cpg	865.73	J/mol×K	1018.16	Joback Method

Sources

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=C64959&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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