Adiphenine

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)18-13-9-6-10-1
InchiKey:	JGOAIQNSOGZNBX-UHFFFAOYSA-N
Formula:	C20H25NO2
SMILES:	CCN(CC)CCOC(=O)C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	311.42

Physical Properties

Property code	Value	Unit	Source
hfus	37.92	kJ/mol	Joback Method
hvap	83.83	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.71		Cheméo Relay (1.0)
logp	3.704		Crippen Method
mcvol	262.560	ml/mol	McGowan Method
rinpol	2186.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2220.00		NIST Webbook

rinpol	2250.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	642.82	K	Cheméo Relay (1.0)
tf	318.04	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64959&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point