Carbetapentane

Other names:	Cyclopentanecarboxylic acid, 1-phenyl-, 2-[2-(diethylamino)ethoxy]ethyl ester Atussil Ethanol, 2-[2-(diethylamino)ethoxy]-, 1-phenylcyclopentanecarboxylate (ester) Pentoxiverin Pentoxyverin Pentoxyverine U.C.B. 2543 1-Phenylcyclopentane-1-Carboxylic acid diethylaminoethoxyethyl ester 2-(Diethylaminoethoxy)ethyl 1-phenyl-1-cyclopentanecarboxylate 2-(Diethylaminoethoxy)ethyl 1-phenylcyclopentyl-1-carboxylate 2-(2-Diethylaminoethoxy)ethyl 1-phenylcyclopentanecarboxylate 2-[2-(Diemthylamino)ethoxy]ethyl 1-phenylcyclopentanecarboxylate Pentoxiverine 1-Cyclopentanecarboxylate, 2-(diethylaminoethoxy)ethyl-1-phenyl-
Inchi:	InChI=1S/C20H31NO3/c1-3-21(4-2)14-15-23-16-17-24-19(22)20(12-8-9-13-20)18-10-6-5
InchiKey:	CFJMRBQWBDQYMK-UHFFFAOYSA-N
Formula:	C20H31NO3
SMILES:	CCN(CC)CCOCCOC(=O)C1(c2ccccc2)CCCC1
Mol. weight [g/mol]:	333.46
CAS:	77-23-6

Physical Properties

Property code	Value	Unit	Source
gf	32.85	kJ/mol	Joback Method
hf	-453.37	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.400		Crippen Method
mcvol	281.330	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	810.35	K	Joback Method

tc	1021.33	K	Joback Method
tf	503.24	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.41	J/mol×K	810.35	Joback Method
cpg	907.43	J/mol×K	845.51	Joback Method
cpg	926.62	J/mol×K	880.68	Joback Method
cpg	945.11	J/mol×K	915.84	Joback Method
cpg	963.03	J/mol×K	951.00	Joback Method
cpg	980.51	J/mol×K	986.16	Joback Method
cpg	997.69	J/mol×K	1021.33	Joback Method

Sources

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=C77236&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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