Cyclopentanecarboxylic acid, 1-phenyl-, 2-(diethylamino)ethyl ester

Other names: Caramiphen
Parpanil
Pentaphen (pharmaceutical)
Parpanit
Pentaphen
1-Phenylcyclopentanecarboxylic acid 2-(diethylamino)ethyl ester
2-Diethylaminoethyl 1-phenylcyclopentane-1-carboxylate
2-Dimethylaminoethyl 1-phenylcyclopentane-1-carboxylate

Inchi: InChI=1S/C18H27NO2/c1-3-19(4-2)14-15-21-17(20)18(12-8-9-13-18)16-10-6-5-7-11-16/h

InchiKey: OFAIGZWCDGNZGT-UHFFFAOYSA-N

Formula: C18H27NO2

SMILES: CCN(CC)CCOC(=O)C1(c2ccccc2)CCCC1

Mol. weight [g/mol]: 289.41

CAS: 77-22-5

Physical Properties

Property code	Value	Unit	Source
gf	121.01	kJ/mol	Joback Method
hf	-279.87	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	68.24	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.383		Crippen Method
mcvol	247.280	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1971.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	742.17	K	Joback Method
tc	959.19	K	Joback Method
tf	458.47	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.39	J/mol×K	742.17	Joback Method
cpg	759.25	J/mol×K	778.34	Joback Method
cpg	778.16	J/mol×K	814.51	Joback Method
cpg	796.24	J/mol×K	850.68	Joback Method
cpg	813.67	J/mol×K	886.85	Joback Method
cpg	830.59	J/mol×K	923.02	Joback Method
cpg	847.16	J/mol×K	959.19	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=C77225&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