Propanidid

Other names:	Benzeneacetic acid, 4-[2-(diethylamino)-2-oxoethoxy]-3-methoxy-, propyl ester Acetic acid, (4-((diethylcarbamoyl)methoxy)-3-methoxyphenyl)-, propyl ester Acetic acid, (p-((diethylcarbamoyl)methoxy)-3-methoxyphenyl)-, propyl ester BAY 1420 Bayer 1420 4-(2-(Diethylamino)-2-oxoethoxy)-3-methoxybenzeneacetic acid propyl ester (p-((Diethylcarbamoyl)methoxy)-3-methoxyphenyl)acetic acid propyl ester (4-((Diethylcarbamoyl)methoxy)-3-methoxyphenyl)acetic acid propyl ester Eponthol Epontol Fabantol Fabontal FBA 1420 (3-Methoxy-4-((N,N-diethylcarbamido)methoxy)phenyl)acetic acid n-propyl ester Propanidide Propantan Propyl(4-((diethylcarbamoyl)methoxy)-3-methoxyphenyl)acetate Sombrevin 2180 TH WH 5668 TH-2180 13245RP
Inchi:	InChI=1S/C18H27NO5/c1-5-10-23-18(21)12-14-8-9-15(16(11-14)22-4)24-13-17(20)19(6-
InchiKey:	KEJXLQUPYHWCNM-UHFFFAOYSA-N
Formula:	C18H27NO5
SMILES:	CCCOC(=O)Cc1ccc(OCC(=O)N(CC)CC)c(OC)c1
Mol. weight [g/mol]:	337.41
CAS:	1421-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-268.23	kJ/mol	Joback Method
hf	-755.55	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method

logp	2.438		Crippen Method
mcvol	271.450	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	835.32	K	Joback Method
tc	1035.83	K	Joback Method
tf	543.10	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.04	J/mol×K	835.32	Joback Method
cpg	846.21	J/mol×K	868.74	Joback Method
cpg	860.26	J/mol×K	902.16	Joback Method
cpg	873.17	J/mol×K	935.58	Joback Method
cpg	884.97	J/mol×K	969.00	Joback Method
cpg	895.66	J/mol×K	1002.42	Joback Method
cpg	905.25	J/mol×K	1035.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1421143&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