Ethamivan

Other names:	Benzamide, N,N-diethyl-4-hydroxy-3-methoxy-
	Vanillamide, N,N-diethyl-
	Analepticon
	Corivanil
	Diethamivan
	Diethylvanillamide
	Emivan
	Etamivan
	Etamivanum
	N,N-Diethylvanillamide
	Romecor
	Sevanil
	Simaron
	Vandid
	Vanillic acid diethylamide
	Vanillic acid N,N-diethylamide
	Ventilone
	3-Methoxy-4-hydroxybenzoic acid diethylamide
	Cardiovamil
	Cardiovanil
	Diethylamide de vanillique
	Sevinal
	Vanillinsaeure-diaethylamid
	NSC-406087
Inchi:	InChI=1S/C12H17NO3/c1-4-13(5-2)12(15)9-6-7-10(14)11(8-9)16-3/h6-8,14H,4-5H2,1-3H
InchiKey:	BQJODPIMMWWMFC-UHFFFAOYSA-N
Formula:	C12H17NO3
SMILES:	CCN(CC)C(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	223.27
CAS:	304-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-124.82	kJ/mol	Joback Method
hf	-420.53	kJ/mol	Joback Method
hfus	32.08	kJ/mol	Joback Method

hvap	69.46	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.883		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	674.97	K	Joback Method
tc	888.60	K	Joback Method
tf	480.29	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.91	J/mol×K	674.97	Joback Method
cpg	498.56	J/mol×K	710.57	Joback Method
cpg	511.39	J/mol×K	746.18	Joback Method
cpg	523.47	J/mol×K	781.78	Joback Method
cpg	534.86	J/mol×K	817.39	Joback Method
cpg	545.62	J/mol×K	852.99	Joback Method
cpg	555.82	J/mol×K	888.60	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C304847&Units=SI

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

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