

DESMETHYLVERAPAMIL

Other names:	Benzeneacetonitrile, «alpha»-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]propyl]-3,4-dimethoxy-«alpha»-(1-methoxy-2-phenylethyl)-1-chloride 67812-42-4 (chloride)
Inchi:	5-[(3,4-dimethoxyphenethyl)amino]-2-(3,4-dimethoxyphenyl)-2-isopropylvaleronitrile
InchiKey:	UPKQNCPPKPOLASS-UHFFFAOYSA-N
Formula:	C26H36N2O4
SMILES:	COc1ccc(CCNCCCC(C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC
Mol. weight [g/mol]:	440.58

Physical Properties

Property code	Value	Unit	Source
hfus	50.04	kJ/mol	Joback Method
log10ws	-4.38		Cheméo Relay (1.0)
logp	4.751		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
tf	432.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.44	J/mol×K	1105.82	Joback Method
cpg	1249.54	J/mol×K	1147.16	Joback Method
cpg	1258.70	J/mol×K	1188.49	Joback Method
cpg	1265.96	J/mol×K	1229.83	Joback Method
cpg	1271.37	J/mol×K	1271.16	Joback Method
cpg	1274.97	J/mol×K	1312.50	Joback Method
cpg	1276.80	J/mol×K	1353.84	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C67018853&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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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