

(+)-2-Methylbutyl p-((p-methoxybenzylidene)amino)cinnamate

Other names:

2-Propenoic acid,
3-[4-[(4-methoxyphenyl)methylene]amino]phenyl]-, 2-methylbutyl ester, [S-(E,E)]-
Propanoic acid, 3-[4-(4-methoxyphenyl)methyleneamino]phenyl]-, 2-methylbutyl
ester, [S-(E,E)]-
Propanoic acid, 3-[4-(4-methoxybenzylideneamino)phenyl]-, 2-methylbutyl ester,
(S)-(+)-
(+)-2-Methylbutyl 4-methoxybenzylidene-4'-aminocinnamate

Inchi:	2-Propenoic acid, 3-[4-[(4-methoxyphenyl)methylene]amino]phenyl]-, 2-methylbutyl ester, [S-(E,E)]- Propanoic acid, 3-[4-(4-methoxyphenyl)methyleneamino]phenyl]-, 2-methylbutyl ester, [S-(E,E)]- InChI=1S/C22H25NO3/c1-4-17(2)16-26-22(24)14-9-18-5-10-20(11-6-18)23-15-19-7-12-2
InchiKey:	FKZXVOQEYXOXAD-IAMGCYTJSA-N
Formula:	C22H25NO3
SMILES:	CCC(C)COC(=O)C=Cc1ccc(N=Cc2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	351.44
CAS:	24140-30-5

Physical Properties

Property code	Value	Unit	Source
hf	-230.15	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.048		Crippen Method
mcvol	288.010	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
tb	945.19	K	Joback Method
tc	1180.64	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24140305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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