

Adipic acid, 3,4-bis(3',4'-dimethoxyphenyl)-, dimethyl ester

Inchi:	InChI=1S/C24H30O8/c1-27-19-9-7-15(11-21(19)29-3)17(13-23(25)31-5)18(14-24(26)32-
InchiKey:	BFGVZIILGIKTHG-UHFFFAOYSA-N
Formula:	C24H30O8
SMILES:	COC(=O)CC(c1ccc(OC)c(OC)c1)C(CC(=O)OC)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	446.49
CAS:	116435-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-555.22	kJ/mol	Joback Method
hf	-1140.55	kJ/mol	Joback Method
hfus	47.72	kJ/mol	Joback Method
hvap	103.39	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.715		Crippen Method
mcvol	339.860	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
tb	1063.18	K	Joback Method
tc	1302.01	K	Joback Method
tf	666.40	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.91	J/molxK	1063.18	Joback Method
cpg	1125.43	J/molxK	1102.99	Joback Method
cpg	1131.47	J/molxK	1142.79	Joback Method
cpg	1134.98	J/molxK	1182.60	Joback Method
cpg	1135.91	J/molxK	1222.40	Joback Method
cpg	1134.23	J/molxK	1262.21	Joback Method
cpg	1129.88	J/molxK	1302.01	Joback Method
dvisc	0.0000682	Paxs	666.40	Joback Method
dvisc	0.0000411	Paxs	732.53	Joback Method

dvisc	0.0000270	Paxs	798.66	Joback Method
dvisc	0.0000189	Paxs	864.79	Joback Method
dvisc	0.0000139	Paxs	930.92	Joback Method
dvisc	0.0000106	Paxs	997.05	Joback Method
dvisc	0.0000084	Paxs	1063.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435600&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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