

(Z)-3,4-Dimethoxycinnamic acid

Inchi:	InChI=1S/C11H12O4/c1-14-9-5-3-8(4-6-11(12)13)7-10(9)15-2/h3-7H,1-2H3,(H,12,13)/b6
InchiKey:	HJBWJAPEBGSQLR-XQRVVYSFSA-N
Formula:	C11H12O4
SMILES:	COc1ccc(C=CC(=O)O)cc1OC
Mol. weight [g/mol]:	208.21

Physical Properties

Property code	Value	Unit	Source
gf	-260.63	kJ/mol	Joback Method
hf	-468.81	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	71.88	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.802		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinqol	1864.00		NIST Webbook
tb	682.77	K	Joback Method
tc	886.19	K	Joback Method
tf	415.32	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.37	J/molxK	682.77	Joback Method
cpg	410.13	J/molxK	716.67	Joback Method
cpg	420.26	J/molxK	750.58	Joback Method
cpg	429.78	J/molxK	784.48	Joback Method
cpg	438.68	J/molxK	818.39	Joback Method
cpg	446.99	J/molxK	852.29	Joback Method
cpg	454.69	J/molxK	886.19	Joback Method
dvisc	0.0009159	Paxs	415.32	Joback Method
dvisc	0.0004082	Paxs	459.89	Joback Method

dvisc	0.0002098	Paxs	504.47	Joback Method
dvisc	0.0001202	Paxs	549.04	Joback Method
dvisc	0.0000748	Paxs	593.62	Joback Method
dvisc	0.0000498	Paxs	638.19	Joback Method
dvisc	0.0000349	Paxs	682.77	Joback Method

Sources

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=R411500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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