

4-Methoxycinnamyl cinnamate

Inchi:	InChI=1S/C19H18O3/c1-21-18-12-9-17(10-13-18)8-5-15-22-19(20)14-11-16-6-3-2-4-7-16
InchiKey:	ZLUKCCCLNLQLQQ-HLSRHWEP-SA-N
Formula:	C19H18O3
SMILES:	COc1ccc(C=CCOC(=O)C=Cc2ccccc2)cc1
Mol. weight [g/mol]:	294.34

Physical Properties

Property code	Value	Unit	Source
gf	145.81	kJ/mol	Joback Method
hf	-116.48	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.965		Crippen Method
mcvol	235.760	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2645.00		NIST Webbook
tb	799.49	K	Joback Method
tc	1034.44	K	Joback Method
tf	453.48	K	Joback Method
vc	0.885	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.26	J/mol×K	799.49	Joback Method
cpg	723.07	J/mol×K	995.28	Joback Method
cpg	712.16	J/mol×K	956.12	Joback Method
cpg	700.30	J/mol×K	916.96	Joback Method
cpg	687.42	J/mol×K	877.81	Joback Method
cpg	673.43	J/mol×K	838.65	Joback Method
cpg	733.11	J/mol×K	1034.44	Joback Method
dvisc	0.0000498	Paxs	799.49	Joback Method
dvisc	0.0000638	Paxs	741.82	Joback Method

dvisc	0.0000854	Paxs	684.15	Joback Method
dvisc	0.0001205	Paxs	626.49	Joback Method
dvisc	0.0001822	Paxs	568.82	Joback Method
dvisc	0.0003026	Paxs	511.15	Joback Method
dvisc	0.0005719	Paxs	453.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
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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