

4-Methoxycinnamyl cinnamate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

ZLUKCCCLNLQLQQ-HLSRHWEP

SA-N

C19H18O3

COc1ccc(C=CCOC(=O)C=Cc2ccccc2)cc1

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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.26	J/mol×K	799.49	Joback Method
cpg	673.43	J/mol×K	838.65	Joback Method
cpg	687.42	J/mol×K	877.81	Joback Method
cpg	700.30	J/mol×K	916.96	Joback Method
cpg	712.16	J/mol×K	956.12	Joback Method
cpg	723.07	J/mol×K	995.28	Joback Method
cpg	733.11	J/mol×K	1034.44	Joback Method
dvisc	0.0005719	Pa×s	453.48	Joback Method
dvisc	0.0003026	Pa×s	511.15	Joback Method

dvisc	0.0001822	Pa×s	568.82	Joback Method
dvisc	0.0001205	Pa×s	626.49	Joback Method
dvisc	0.0000854	Pa×s	684.15	Joback Method
dvisc	0.0000638	Pa×s	741.82	Joback Method
dvisc	0.0000498	Pa×s	799.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55654&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
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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