

Methyl cis-cinnamate

Inchi:	InChI=1S/C10H10O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7+
InchiKey:	CCRCUPLGCSFEDV-FPLPWBNLSA-N
Formula:	C10H10O2
SMILES:	COC(=O)/C=C\c1ccccc1
Mol. weight [g/mol]:	162.19

Physical Properties

Property code	Value	Unit	Source
af	0.4397		Cheméo Relay (1.0)
hf	-197.71	kJ/mol	Cheméo Relay (1.0)
hfus	18.69	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-2.58		Cheméo Relay (1.0)
logp	1.873		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1308.20		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1308.20		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1281.00		NIST Webbook
tb	520.05	K	Cheméo Relay (1.0)

tc	709.57	K	Cheméo Relay (1.0)
tf	262.81	K	Cheméo Relay (1.0)
vc	0.458	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.89	J/mol×K	535.33	Joback Method
cpg	294.93	J/mol×K	572.44	Joback Method
cpg	307.12	J/mol×K	609.55	Joback Method
cpg	318.52	J/mol×K	646.66	Joback Method
cpg	329.15	J/mol×K	683.77	Joback Method
cpg	339.04	J/mol×K	720.88	Joback Method
cpg	348.24	J/mol×K	757.99	Joback Method
dvisc	0.0021489	Pa×s	295.96	Joback Method
dvisc	0.0011171	Pa×s	335.86	Joback Method
dvisc	0.0006673	Pa×s	375.75	Joback Method
dvisc	0.0004400	Pa×s	415.64	Joback Method
dvisc	0.0003121	Pa×s	455.54	Joback Method
dvisc	0.0002340	Pa×s	495.43	Joback Method
dvisc	0.0001831	Pa×s	535.33	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19713736&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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