trans-3-methoxycinnamic acid

Other names:	2-Propenoic acid, 3-(3-methoxyphenyl)-
	3-(3-Methoxyphenyl)acrylic acid
	Cinnamic acid, m-methoxy-
	Propenoic acid, 3-(3-methoxyphenyl)-, trans-
	m-Methoxycinnamic acid
	trans-3-Methoxycinnamic acid
Inchi:	InChI=1S/C10H10O3/c1-13-9-4-2-3-8(7-9)5-6-10(11)12/h2-7H,1H3,(H,11,12)
InchiKey:	LZPNXAULYJPXEH-AATRIKPKSA-N
Formula:	C10H10O3
SMILES:	COc1cccc(C=CC(=O)O)c1
Mol. weight [g/mol]:	178.18
CAS:	17570-26-2

Physical Properties

Property code	Value	Unit	Source
hf	-386.41	kJ/mol	Cheméo Relay (1.0)
hfus	22.39	kJ/mol	Joback Method
hsub	124.00 ± 0.90	kJ/mol	NIST Webbook
hvap	96.96	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	1.793		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
tb	593.04	K	Cheméo Relay (1.0)
tc	788.32	K	Cheméo Relay (1.0)
tf	372.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.56	J/mol×K	632.49	Joback Method
cpg	338.85	J/mol×K	667.04	Joback Method
cpg	348.51	J/mol×K	701.59	Joback Method
cpg	357.56	J/mol×K	736.14	Joback Method

cpg	366.02	J/mol×K	770.69	Joback Method
cpg	373.93	J/mol×K	805.24	Joback Method
cpg	381.31	J/mol×K	839.79	Joback Method
dvisc	0.0023160	Pa×s	369.30	Joback Method
dvisc	0.0008973	Pa×s	413.17	Joback Method
dvisc	0.0004170	Pa×s	457.03	Joback Method
dvisc	0.0002217	Pa×s	500.89	Joback Method
dvisc	0.0001304	Pa×s	544.76	Joback Method
dvisc	0.0000831	Pa×s	588.62	Joback Method
dvisc	0.0000563	Pa×s	632.49	Joback Method

Sources

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=C17570262&Units=SI
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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

Latest version available from: