BENZOIC ACID, 4-METHYL-, METHYL ESTER

Other names:	4-(Methoxycarbonyl)toluene
	4-Methylbenzoic acid, methyl ester
	Methyl 4-toluate
	Methyl ester of 4-methylbenzoic acid
	Methyl p-toluenecarboxylate
	NSC 24761
	methyl 4-methylbenzoate
	methyl p-methylbenzoate
	methyl p-toluate
	p-(Methoxycarbonyl)toluene
	p-Carbomethoxytoluene
	p-Toluylic acid, methyl ester
	p-toluic acid, methyl ester
Inchi:	InChI=1S/C9H10O2/c1-7-3-5-8(6-4-7)9(10)11-2/h3-6H,1-2H3
InchiKey:	QSSJZLPUHJDYKF-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	150.18

Physical Properties

Property code	Value	Unit	Source
af	0.4906		Cheméo Relay (1.0)
affp	861.50	kJ/mol	NIST Webbook
basg	830.60	kJ/mol	NIST Webbook
gf	-106.24	kJ/mol	Joback Method
hf	-312.60 ± 6.70	kJ/mol	NIST Webbook
hfs	-393.30 ± 2.40	kJ/mol	NIST Webbook
hfus	20.20	kJ/mol	Vapor Pressures and Phase Diagrams of Two Methyl Esters of Substituted Benzoic Acids
hsub	83.30 ± 0.30	kJ/mol	NIST Webbook
hsub	80.60 ± 6.30	kJ/mol	NIST Webbook
hsub	80.70	kJ/mol	NIST Webbook
hvap	64.54	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	NIST Webbook
ie	8.94 ± 0.04	eV	NIST Webbook
ie	8.40	eV	NIST Webbook

log10ws	-2.63		Cheméo Relay (1.0)
logp	1.782		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	205.66		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1215.60		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1215.60		NIST Webbook
rinpol	1215.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	489.97	K	Cheméo Relay (1.0)
tc	694.16	K	Cheméo Relay (1.0)
tf	312.32	K	Cheméo Relay (1.0)
vc	0.445	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.24	J/mol×K	513.27	Joback Method
cpg	268.48	J/mol×K	549.50	Joback Method
cpg	280.07	J/mol×K	585.73	Joback Method
cpg	291.03	J/mol×K	621.95	Joback Method
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
dvisc	0.0010297	Pa×s	337.45	Joback Method
dvisc	0.0017319	Pa×s	302.29	Joback Method
dvisc	0.0006754	Pa×s	372.62	Joback Method
dvisc	0.0004764	Pa×s	407.78	Joback Method
dvisc	0.0003552	Pa×s	442.94	Joback Method
dvisc	0.0002765	Pa×s	478.11	Joback Method
dvisc	0.0002227	Pa×s	513.27	Joback Method
hfust	20.78	kJ/mol	162.50	NIST Webbook
hfust	20.77	kJ/mol	306.50	NIST Webbook
hsubt	51.60	kJ/mol	448.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99752&Units=SI
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):	
Vapor Pressures and Phase Diagrams of Two Methyl Esters of Substituted Benzoic Acids:	https://www.doi.org/10.1021/je2007605

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume