Benzoic acid, 3-methyl-, methyl ester

Other names:	m-Toluic acid, methyl ester
	Methyl m-methylbenzoate
	Methyl m-toluate
	Methyl 3-methylbenzoate
	Methyl 3-toluate
	3-Methylbenzoic acid, methyl ester
	meta-Toluic acid, methyl ester
	m-Toluylic acid, methyl ester
Inchi:	InChI=1S/C9H10O2/c1-7-4-3-5-8(6-7)9(10)11-2/h3-6H,1-2H3
InchiKey:	CPXCDEMFNPKOEF-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	150.17
CAS:	99-36-5

Physical Properties

Property code	Value	Unit	Source
affp	857.70	kJ/mol	NIST Webbook
basg	826.80	kJ/mol	NIST Webbook
gf	-106.24	kJ/mol	Joback Method
hf	-248.83	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.782		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1171.00		NIST Webbook
rinpol	1205.70		NIST Webbook
rinpol	203.97		NIST Webbook
rinpol	1205.70		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	203.97		NIST Webbook
rinpol	1235.00		NIST Webbook

rinpol	1190.00		NIST Webbook
ripol	1744.00		NIST Webbook
tb	513.27	K	Joback Method
tc	730.64	K	Joback Method
tf	302.29	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
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
dvisc	0.0003552	Pa×s	442.94	Joback Method
dvisc	0.0002227	Pa×s	513.27	Joback Method
dvisc	0.0002765	Pa×s	478.11	Joback Method
dvisc	0.0017319	Pa×s	302.29	Joback Method
dvisc	0.0010297	Pa×s	337.45	Joback Method
dvisc	0.0006754	Pa×s	372.62	Joback Method
dvisc	0.0004764	Pa×s	407.78	Joback Method
hfust	21.15	kJ/mol	269.90	NIST Webbook
hfust	17.14	kJ/mol	162.50	NIST Webbook
hvapt	53.50	kJ/mol	388.00	NIST Webbook
hvapt	54.80	kJ/mol	429.50	NIST Webbook
hvapt	60.30 ± 0.20	kJ/mol	296.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	3.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99365&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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