Benzeneacetic acid, methyl ester

Other names:	Acetic acid, phenyl-, methyl ester
	Methyl «alpha»-toluate
	Methyl benzeneacetate
	Methyl phenylacetate
	Methyl 2-phenylacetate
	Phenylacetic acid, methyl ester
	Methyl ester of phenylacetic acid
	Mephaneine
	Methyl phenylethanoate
	Methyl benzeneethanoate
	NSC 401667
Inchi:	InChI=1S/C9H10O2/c1-11-9(10)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	CRZQGDNQQAALAY-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COC(=O)Cc1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	101-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-96.61	kJ/mol	Joback Method
hf	-237.36	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	57.40	kJ/mol	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.402		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1140.48		NIST Webbook
rinpol	1142.07		NIST Webbook
rinpol	1143.76		NIST Webbook
rinpol	1148.60		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1186.00		NIST Webbook

rinpol	1179.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1193.60	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1180.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1178.90	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1139.02	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1194.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1176.00	NIST Webbook
rinpol	1160.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1193.60	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1158.70	NIST Webbook
rinpol	1149.00	NIST Webbook

rinpol	1186.00		NIST Webbook
rinpol	1156.39		NIST Webbook
rinpol	1154.04		NIST Webbook
rinpol	1151.74		NIST Webbook
rinpol	1149.57		NIST Webbook
rinpol	1147.51		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1145.60		NIST Webbook
rinpol	1149.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	491.20	K	NIST Webbook
tc	724.46	K	Joback Method
tf	289.77	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.39	J/mol×K	508.29	Joback Method
cpg	269.00	J/mol×K	544.32	Joback Method
cpg	280.90	J/mol×K	580.35	Joback Method
cpg	292.11	J/mol×K	616.37	Joback Method
cpg	302.63	J/mol×K	652.40	Joback Method
cpg	312.50	J/mol×K	688.43	Joback Method
cpg	321.72	J/mol×K	724.46	Joback Method

dvisc	0.0023343	Pa×s	289.77	Joback Method
dvisc	0.0012799	Pa×s	326.19	Joback Method
dvisc	0.0007918	Pa×s	362.61	Joback Method
dvisc	0.0005347	Pa×s	399.03	Joback Method
dvisc	0.0003856	Pa×s	435.45	Joback Method
dvisc	0.0002925	Pa×s	471.87	Joback Method
dvisc	0.0002308	Pa×s	508.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.70	K	6.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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