Benzenebutanoic acid, methyl ester

Other names:	Butyric acid, 4-phenyl-, methyl ester
	Methyl 4-phenylbutanoate
	Methyl 4-phenylbutyrate
	Methyl ester of benzenebutanoic acid
	4-Phenylbutanoic acid methyl ester
Inchi:	InChI=1S/C11H14O2/c1-13-11(12)9-5-8-10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3
InchiKey:	YRYZGVBKMWFWGT-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	COC(=O)CCCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	2046-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
ie	8.60 ± 0.30	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/mol×K	554.05	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
cpg	374.48	J/mol×K	623.81	Joback Method

cpg	387.33	J/mol×K	658.68	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	410.76	J/mol×K	728.44	Joback Method
cpg	421.37	J/mol×K	763.32	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method
dvisc	0.0012165	Pa×s	352.60	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0002006	Pa×s	554.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.00	K	2.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2046175&Units=SI

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume