Benzoic acid, 2,4,6-trimethyl-, methyl ester

Other names:	Methyl «beta»-isodurilate
	Methyl mesitoate
	Methyl 2,4,6-trimethylbenzoate
	2,4,6-(CH3)3-C6H2-COOCH3
Inchi:	InChI=1S/C11H14O2/c1-7-5-8(2)10(9(3)6-7)11(12)13-4/h5-6H,1-4H3
InchiKey:	PXLABDTXHJPRRH-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	COC(=O)c1c(C)cc(C)cc1C
Mol. weight [g/mol]:	178.23
CAS:	2282-84-0

Physical Properties

Property code	Value	Unit	Source
affp	866.30	kJ/mol	NIST Webbook
basg	835.30	kJ/mol	NIST Webbook
gf	-108.66	kJ/mol	Joback Method
hf	-313.05	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.398		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	230.42		NIST Webbook
rinpol	1311.00		NIST Webbook
tb	568.99	K	Joback Method
tc	781.39	K	Joback Method
tf	349.87	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	345.39	J/mol×K	568.99	Joback Method
cpg	359.01	J/mol×K	604.39	Joback Method
cpg	371.96	J/mol×K	639.79	Joback Method
cpg	384.25	J/mol×K	675.19	Joback Method
cpg	395.89	J/mol×K	710.59	Joback Method
cpg	406.88	J/mol×K	745.99	Joback Method
cpg	417.21	J/mol×K	781.39	Joback Method
dvisc	0.0010802	Pa×s	349.87	Joback Method
dvisc	0.0007022	Pa×s	386.39	Joback Method
dvisc	0.0004918	Pa×s	422.91	Joback Method
dvisc	0.0003644	Pa×s	459.43	Joback Method
dvisc	0.0002823	Pa×s	495.95	Joback Method
dvisc	0.0002264	Pa×s	532.47	Joback Method
dvisc	0.0001868	Pa×s	568.99	Joback Method

Sources

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=C2282840&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume