1,3-Benzenedicarboxylic acid, monomethyl ester

Other names: Isophthalic acid, monomethyl ester
Methyl hydrogen isophthalate
Monomethyl isophthalate

Inchi: InChI=1S/C9H8O4/c1-13-9(12)7-4-2-3-6(5-7)8(10)11/h2-5H,1H3,(H,10,11)

InchiKey: WMZNGTSLFSJHMZ-UHFFFAOYSA-N

Formula: C9H8O4

SMILES: COC(=O)c1cccc(C(=O)O)c1

Mol. weight [g/mol]: 180.16

CAS: 1877-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-513.64	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Vapor Pressures and Phase Changes Enthalpy and Gibbs Energy of Three Crystalline Monomethyl Benzenedicarboxylates
hsub	125.60 ± 1.00	kJ/mol	NIST Webbook
hvap	71.15	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.171		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	659.32	K	Joback Method
tc	868.49	K	Joback Method
tf	413.04	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.88	J/mol×K	868.49	Joback Method

cpg	313.39	J/mol×K	659.32	Joback Method
cpg	322.42	J/mol×K	694.18	Joback Method
cpg	330.85	J/mol×K	729.04	Joback Method
cpg	338.71	J/mol×K	763.90	Joback Method
cpg	346.00	J/mol×K	798.77	Joback Method
cpg	352.72	J/mol×K	833.63	Joback Method
dvisc	0.0000688	Pa×s	659.32	Joback Method
dvisc	0.0015914	Pa×s	413.04	Joback Method
dvisc	0.0007440	Pa×s	454.09	Joback Method
dvisc	0.0003946	Pa×s	495.13	Joback Method
dvisc	0.0002306	Pa×s	536.18	Joback Method
dvisc	0.0001455	Pa×s	577.23	Joback Method
dvisc	0.0000976	Pa×s	618.27	Joback Method
hfust	36.50	kJ/mol	466.70	NIST Webbook
hsubt	122.60 ± 0.70	kJ/mol	369.00	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=C1877710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Phase Changes Enthalpy and Gibbs Energy of Three Crystalline Monomethyl Benzenedicarboxylates:	https://www.doi.org/10.1021/je0503305

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