Methyl hydrogen phthalate

Other names:	1,2-Benzenedicarboxylic acid, monomethyl ester
	D 3
	D 3 (ester)
	NSC 8281
	Phthalic acid, methyl ester
	monomethyl 1,2-benzenedicarboxylate
	monomethyl phthalate
	o-(Methoxycarbonyl)benzoic acid
	phthalic acid, monomethyl ester
Inchi:	InChI=1S/C9H8O4/c1-13-9(12)7-5-3-2-4-6(7)8(10)11/h2-5H,1H3,(H,10,11)
InchiKey:	FNJSWIPFHMKRAT-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	COC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	180.16
CAS:	4376-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-513.64	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Vapor Pressures and Phase Changes Enthalpy and Gibbs Energy of Three Crystalline Monomethyl Benzenedicarboxylates
hsub	117.90 ± 0.80	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	352.72	J/mol×K	833.63	Joback Method
cpg	346.00	J/mol×K	798.77	Joback Method
cpg	338.71	J/mol×K	763.90	Joback Method
cpg	330.85	J/mol×K	729.04	Joback Method
cpg	322.42	J/mol×K	694.18	Joback Method
cpg	313.39	J/mol×K	659.32	Joback Method
cpg	358.88	J/mol×K	868.49	Joback Method
dvisc	0.0015914	Pa×s	413.04	Joback Method
dvisc	0.0000688	Pa×s	659.32	Joback Method
dvisc	0.0000976	Pa×s	618.27	Joback Method
dvisc	0.0001455	Pa×s	577.23	Joback Method
dvisc	0.0002306	Pa×s	536.18	Joback Method
dvisc	0.0003946	Pa×s	495.13	Joback Method
dvisc	0.0007440	Pa×s	454.09	Joback Method
hfust	21.63	kJ/mol	357.50	NIST Webbook
hsubt	115.90 ± 0.60	kJ/mol	345.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4376185&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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