

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.72	J/molxK	833.63	Joback Method
cpg	346.00	J/molxK	798.77	Joback Method
cpg	338.71	J/molxK	763.90	Joback Method
cpg	330.85	J/molxK	729.04	Joback Method
cpg	322.42	J/molxK	694.18	Joback Method
cpg	313.39	J/molxK	659.32	Joback Method
cpg	358.88	J/molxK	868.49	Joback Method
dvisc	0.0015914	Paxs	413.04	Joback Method
dvisc	0.0000688	Paxs	659.32	Joback Method
dvisc	0.0000976	Paxs	618.27	Joback Method
dvisc	0.0001455	Paxs	577.23	Joback Method
dvisc	0.0002306	Paxs	536.18	Joback Method
dvisc	0.0003946	Paxs	495.13	Joback Method
dvisc	0.0007440	Paxs	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

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 Polymers	https://www.doi.org/10.1021/je0503305
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Benzene dicarboxylates: McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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