1,2-Benzenedicarboxylic acid, 4-methyl-

Other names: Phthalic acid, 4-methyl-
4-Methyl-1,2-benzenedicarboxylic acid
4-Methylphthalic acid
Inchi: InChI=1S/C9H8O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13)
InchiKey: CWJJAFQCTXFSTA-UHFFFAOYSA-N
Formula: C9H8O4
SMILES: Cc1ccc(C(=O)O)c(C(=O)O)c1
Mol. weight [g/mol]: 180.16
CAS: 4316-23-8

Physical Properties

Property code	Value	Unit	Source
gf	-413.43	kJ/mol	Joback Method
hf	-545.12	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	86.08	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.391		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
rinpol	247.15		NIST Webbook
tb	734.06	K	Joback Method
tc	934.41	K	Joback Method
tf	464.15	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.42	J/mol×K	734.06	Joback Method
cpg	336.65	J/mol×K	767.45	Joback Method
cpg	343.39	J/mol×K	800.84	Joback Method
cpg	349.67	J/mol×K	834.24	Joback Method
cpg	355.49	J/mol×K	867.63	Joback Method

cpg	360.87	J/mol×K	901.02	Joback Method
cpg	365.83	J/mol×K	934.41	Joback Method
dvisc	0.0008293	Pa×s	464.15	Joback Method
dvisc	0.0003189	Pa×s	509.13	Joback Method
dvisc	0.0001432	Pa×s	554.12	Joback Method
dvisc	0.0000725	Pa×s	599.11	Joback Method
dvisc	0.0000404	Pa×s	644.09	Joback Method
dvisc	0.0000243	Pa×s	689.07	Joback Method
dvisc	0.0000155	Pa×s	734.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4316238&Units=SI
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

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
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