1,4-Benzenedicarboxaldehyde, 2-methyl-

Other names: Terephthalaldehyde, methyl-
2-Methylterephthalaldehyde
2-Methyl-p-phthalaldehyde
Inchi: InChI=1S/C9H8O2/c1-7-4-8(5-10)2-3-9(7)6-11/h2-6H,1H3
InchiKey: MNHWRUCVFATHDL-UHFFFAOYSA-N
Formula: C9H8O2
SMILES: Cc1cc(C=O)ccc1C=O
Mol. weight [g/mol]: 148.16
CAS: 27587-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-80.99	kJ/mol	Joback Method
hf	-186.66	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.620		Crippen Method
mcvol	117.050	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	539.28	K	Joback Method
tc	758.36	K	Joback Method
tf	326.65	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.21	J/mol×K	539.28	Joback Method
cpg	260.57	J/mol×K	575.79	Joback Method
cpg	270.31	J/mol×K	612.31	Joback Method
cpg	279.45	J/mol×K	648.82	Joback Method
cpg	288.01	J/mol×K	685.33	Joback Method
cpg	296.01	J/mol×K	721.84	Joback Method

cpg	303.47	J/mol×K	758.36	Joback Method
dvisc	0.0020171	Pa×s	326.65	Joback Method
dvisc	0.0012969	Pa×s	362.09	Joback Method
dvisc	0.0009022	Pa×s	397.53	Joback Method
dvisc	0.0006660	Pa×s	432.96	Joback Method
dvisc	0.0005148	Pa×s	468.40	Joback Method
dvisc	0.0004126	Pa×s	503.84	Joback Method
dvisc	0.0003404	Pa×s	539.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27587173&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
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
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