

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:	<chem>Cc1cc(C=O)ccc1C=O</chem>
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/molxK	539.28	Joback Method
cpg	260.57	J/molxK	575.79	Joback Method
cpg	270.31	J/molxK	612.31	Joback Method
cpg	279.45	J/molxK	648.82	Joback Method
cpg	288.01	J/molxK	685.33	Joback Method
cpg	296.01	J/molxK	721.84	Joback Method

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27587173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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