P-PHENYLENEDIACETIC ACID

Other names: p-Phenylenediacetic acid
p-Benzenediacetic acid
1,4-Benzenediacetic acid
Inchi: InChI=1S/C10H10O4/c11-9(12)5-7-1-2-8(4-3-7)6-10(13)14/h1-4H,5-6H2,(H,11,12)(H,13,
InchiKey: SLWIPPZWFZGHEU-UHFFFAOYSA-N
Formula: C10H10O4
SMILES: O=C(O)Cc1ccc(CC(=O)O)cc1
Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
hf	-698.78	kJ/mol	Cheméo Relay (1.0)
hfus	26.68	kJ/mol	Joback Method
hvap	111.12	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-1.66		Cheméo Relay (1.0)
logp	0.941		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	571.70	K	Cheméo Relay (1.0)
tf	458.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.29	J/mol×K	751.96	Joback Method
cpg	389.27	J/mol×K	784.98	Joback Method
cpg	396.71	J/mol×K	817.99	Joback Method
cpg	403.63	J/mol×K	851.01	Joback Method
cpg	410.06	J/mol×K	884.02	Joback Method
cpg	416.01	J/mol×K	917.04	Joback Method
cpg	421.52	J/mol×K	950.05	Joback Method
dvisc	0.0009400	Pa×s	462.90	Joback Method
dvisc	0.0003283	Pa×s	511.08	Joback Method

dvisc	0.0001374	Pa×s	559.25	Joback Method
dvisc	0.0000661	Pa×s	607.43	Joback Method
dvisc	0.0000354	Pa×s	655.61	Joback Method
dvisc	0.0000206	Pa×s	703.78	Joback Method
dvisc	0.0000129	Pa×s	751.96	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7325464&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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