BENZENEACETIC ACID, 2,4-DIMETHYL-

Other names: 2,4-Dimethylphenylacetic acid
Inchi: InChI=1S/C10H12O2/c1-7-3-4-9(6-10(11)12)8(2)5-7/h3-5H,6H2,1-2H3,(H,11,12)
InchiKey: MWBXCWLRASBZFB-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: Cc1ccc(CC(=O)O)c(C)c1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
af	0.7042		Cheméo Relay (1.0)
chs	-5150.10	kJ/mol	NIST Webbook
gf	-139.27	kJ/mol	Joback Method
hf	-385.05	kJ/mol	Cheméo Relay (1.0)
hfs	-504.20	kJ/mol	NIST Webbook
hfus	20.61	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-2.08		Cheméo Relay (1.0)
logp	1.931		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	558.00	K	Cheméo Relay (1.0)
tc	776.35	K	Cheméo Relay (1.0)
tf	370.28	K	Cheméo Relay (1.0)
vc	0.481	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.71	J/mol×K	610.89	Joback Method
cpg	382.32	J/mol×K	813.03	Joback Method
cpg	374.26	J/mol×K	779.34	Joback Method
cpg	365.68	J/mol×K	745.65	Joback Method
cpg	356.56	J/mol×K	711.96	Joback Method

cpg	346.86	J/mol×K	678.27	Joback Method
cpg	336.59	J/mol×K	644.58	Joback Method
dvisc	0.0003160	Pa×s	487.78	Joback Method
dvisc	0.0000861	Pa×s	610.89	Joback Method
dvisc	0.0001247	Pa×s	569.85	Joback Method
dvisc	0.0001915	Pa×s	528.82	Joback Method
dvisc	0.0027935	Pa×s	364.67	Joback Method
dvisc	0.0005718	Pa×s	446.74	Joback Method
dvisc	0.0011664	Pa×s	405.71	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6331040&Units=SI

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):

Legend

af: Acentric Factor
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume