2,3,5,6-Tetramethylbenzoic acid

Other names: Benzoic acid, 2,3,5,6-tetramethyl-
Inchi: InChI=1S/C11H14O2/c1-6-5-7(2)9(4)10(8(6)3)11(12)13/h5H,1-4H3,(H,12,13)
InchiKey: STIDRZRESMTQBD-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: Cc1cc(C)c(C)c(C(=O)O)c1C
Mol. weight [g/mol]: 178.23
CAS: 2604-45-7

Physical Properties

Property code	Value	Unit	Source
chs	-5823.50 ± 1.00	kJ/mol	NIST Webbook
gf	-150.11	kJ/mol	Joback Method
hf	-400.10 ± 2.20	kJ/mol	NIST Webbook
hf	-400.00	kJ/mol	NIST Webbook
hfs	-506.10 ± 1.00	kJ/mol	NIST Webbook
hfs	-506.20 ± 2.00	kJ/mol	NIST Webbook
hfus	22.42	kJ/mol	Joback Method
hsub	106.10 ± 0.80	kJ/mol	NIST Webbook
hsub	106.10 ± 0.80	kJ/mol	NIST Webbook
hsub	106.10	kJ/mol	NIST Webbook
hvap	68.43	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.618		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	643.73	K	Joback Method
tc	844.89	K	Joback Method
tf	400.98	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.49	J/mol×K	643.73	Joback Method

cpg	382.80	J/mol×K	677.26	Joback Method
cpg	393.53	J/mol×K	710.78	Joback Method
cpg	403.70	J/mol×K	744.31	Joback Method
cpg	413.31	J/mol×K	777.84	Joback Method
cpg	422.39	J/mol×K	811.36	Joback Method
cpg	430.93	J/mol×K	844.89	Joback Method
cps	231.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0013439	Pa×s	400.98	Joback Method
dvisc	0.0006556	Pa×s	441.44	Joback Method
dvisc	0.0003608	Pa×s	481.90	Joback Method
dvisc	0.0002178	Pa×s	522.36	Joback Method
dvisc	0.0001414	Pa×s	562.81	Joback Method
dvisc	0.0000972	Pa×s	603.27	Joback Method
dvisc	0.0000701	Pa×s	643.73	Joback Method
hsubt	104.60 ± 0.80	kJ/mol	340.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2604457&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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