Benzoic acid, 2,6-dimethyl-

Other names: 2,6-Dimethylbenzoic acid
Inchi: InChI=1S/C9H10O2/c1-6-4-3-5-7(2)8(6)9(10)11/h3-5H,1-2H3,(H,10,11)
InchiKey: HCBHQDKBSKYGCK-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: Cc1cccc(C)c1C(=O)O
Mol. weight [g/mol]: 150.17
CAS: 632-46-2

Physical Properties

Property code	Value	Unit	Source
chs	-4530.10 ± 0.79	kJ/mol	NIST Webbook
gf	-147.69	kJ/mol	Joback Method
hf	-341.60	kJ/mol	NIST Webbook
hf	-341.60 ± 1.70	kJ/mol	NIST Webbook
hfs	-440.70 ± 1.70	kJ/mol	NIST Webbook
hfs	-440.70 ± 0.96	kJ/mol	NIST Webbook
hfus	18.02	kJ/mol	Joback Method
hsub	99.10 ± 0.20	kJ/mol	NIST Webbook
hsub	99.10	kJ/mol	NIST Webbook
hsub	106.40 ± 0.30	kJ/mol	NIST Webbook
hsub	99.10 ± 0.20	kJ/mol	NIST Webbook
hvap	62.65	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.002		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	588.01	K	Joback Method
tc	793.17	K	Joback Method
tf	353.40	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.47	J/mol×K	793.17	Joback Method
cpg	324.08	J/mol×K	758.97	Joback Method
cpg	279.40	J/mol×K	588.01	Joback Method
cpg	289.42	J/mol×K	622.20	Joback Method
cpg	298.88	J/mol×K	656.40	Joback Method
cpg	307.80	J/mol×K	690.59	Joback Method
cpg	316.19	J/mol×K	724.78	Joback Method
cps	204.20	J/mol×K	299.65	NIST Webbook
dvisc	0.0001000	Pa×s	588.01	Joback Method
dvisc	0.0001448	Pa×s	548.91	Joback Method
dvisc	0.0031453	Pa×s	353.40	Joback Method
dvisc	0.0013296	Pa×s	392.50	Joback Method
dvisc	0.0006569	Pa×s	431.60	Joback Method
dvisc	0.0003649	Pa×s	470.70	Joback Method
dvisc	0.0002218	Pa×s	509.81	Joback Method
hsubt	104.50 ± 0.30	kJ/mol	336.00	NIST Webbook
hsubt	98.20 ± 0.20	kJ/mol	316.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66357e+01
Coeff. B	-5.42303e+03
Coeff. C	-9.33970e+01
Temperature range (K), min.	389.15
Temperature range (K), max.	572.29

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C632462&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume