Benzoic acid, 2,4-dimethyl-

Other names:	2,4-Dimethylbenzoic acid
	4-Carboxy-1,3-dimethylbenzene
Inchi:	InChI=1S/C9H10O2/c1-6-3-4-8(9(10)11)7(2)5-6/h3-5H,1-2H3,(H,10,11)
InchiKey:	BKYWPNROPGQIFZ-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	Cc1ccc(C(=O)O)c(C)c1
Mol. weight [g/mol]:	150.17
CAS:	611-01-8

Physical Properties

Property code	Value	Unit	Source
chs	-4512.32 ± 0.84	kJ/mol	NIST Webbook
gf	-147.69	kJ/mol	Joback Method
hf	-355.00	kJ/mol	NIST Webbook
hf	-355.00 ± 1.70	kJ/mol	NIST Webbook
hfs	-458.50 ± 1.00	kJ/mol	NIST Webbook
hfs	-458.50 ± 1.70	kJ/mol	NIST Webbook
hfus	18.02	kJ/mol	Joback Method
hsub	103.50 ± 0.30	kJ/mol	NIST Webbook
hsub	103.50 ± 0.30	kJ/mol	NIST Webbook
hsub	103.50	kJ/mol	NIST Webbook
hvap	62.65	kJ/mol	Joback Method
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	316.19	J/mol×K	724.78	Joback Method
cpg	307.80	J/mol×K	690.59	Joback Method
cpg	298.88	J/mol×K	656.40	Joback Method
cpg	289.42	J/mol×K	622.20	Joback Method
cpg	279.40	J/mol×K	588.01	Joback Method
cps	192.20	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	0.0002218	Pa×s	509.81	Joback Method
dvisc	0.0003649	Pa×s	470.70	Joback Method
dvisc	0.0006569	Pa×s	431.60	Joback Method
dvisc	0.0013296	Pa×s	392.50	Joback Method
dvisc	0.0031453	Pa×s	353.40	Joback Method
hsubt	102.70 ± 0.30	kJ/mol	321.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	540.20	K	96.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63425e+01
Coeff. B	-5.27132e+03
Coeff. C	-9.15900e+01
Temperature range (K), min.	419.92
Temperature range (K), max.	569.45

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611018&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
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume