Benzoic acid, 2,4,5-trimethyl-

Other names:	2,4,5-Trimethylbenzoic acid
	Durylic acid
Inchi:	InChI=1S/C10H12O2/c1-6-4-8(3)9(10(11)12)5-7(6)2/h4-5H,1-3H3,(H,11,12)
InchiKey:	QENJZWZWAWWESF-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	Cc1cc(C)c(C(=O)O)cc1C
Mol. weight [g/mol]:	164.20
CAS:	528-90-5

Physical Properties

Property code	Value	Unit	Source
chs	-5154.50 ± 1.30	kJ/mol	NIST Webbook
gf	-148.90	kJ/mol	Joback Method
hf	-386.20 ± 2.10	kJ/mol	NIST Webbook
hfs	-495.80 ± 2.00	kJ/mol	NIST Webbook
hfus	20.22	kJ/mol	Joback Method
hsub	109.60	kJ/mol	NIST Webbook
hsub	109.60 ± 0.50	kJ/mol	NIST Webbook
hsub	109.60 ± 0.50	kJ/mol	NIST Webbook
hvap	65.54	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.310		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	615.87	K	Joback Method
tc	818.94	K	Joback Method
tf	377.19	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.55	J/mol×K	818.94	Joback Method
cpg	324.63	J/mol×K	615.87	Joback Method

cpg	335.32	J/mol×K	649.71	Joback Method
cpg	345.44	J/mol×K	683.56	Joback Method
cpg	355.00	J/mol×K	717.40	Joback Method
cpg	364.04	J/mol×K	751.25	Joback Method
cpg	372.55	J/mol×K	785.09	Joback Method
dvisc	0.0000834	Pa×s	615.87	Joback Method
dvisc	0.0020113	Pa×s	377.19	Joback Method
dvisc	0.0009188	Pa×s	416.97	Joback Method
dvisc	0.0004811	Pa×s	456.75	Joback Method
dvisc	0.0002795	Pa×s	496.53	Joback Method
dvisc	0.0001759	Pa×s	536.31	Joback Method
dvisc	0.0001181	Pa×s	576.09	Joback Method
hsubt	108.30 ± 0.50	kJ/mol	335.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36366e+01
Coeff. B	-4.26807e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	408.22
Temperature range (K), max.	601.16

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C528905&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume