Pentamethylbenzoic acid

Other names: Benzoic acid, pentamethyl-
Inchi: InChI=1S/C12H16O2/c1-6-7(2)9(4)11(12(13)14)10(5)8(6)3/h1-5H3,(H,13,14)
InchiKey: MNLKGWIYXCKWBU-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1c(C)c(C)c(C(=O)O)c(C)c1C
Mol. weight [g/mol]: 192.25
CAS: 2243-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-151.32	kJ/mol	Joback Method
hf	-422.90 ± 2.90	kJ/mol	NIST Webbook
hfs	-536.30 ± 2.30	kJ/mol	NIST Webbook
hfus	24.62	kJ/mol	Joback Method
hsub	113.40 ± 1.80	kJ/mol	NIST Webbook
hsub	113.40	kJ/mol	NIST Webbook
hsub	113.40 ± 1.80	kJ/mol	NIST Webbook
hvap	71.32	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.927		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	671.59	K	Joback Method
tc	871.10	K	Joback Method
tf	424.77	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.94	J/mol×K	671.59	Joback Method
cpg	431.82	J/mol×K	704.84	Joback Method
cpg	443.12	J/mol×K	738.09	Joback Method
cpg	453.84	J/mol×K	771.35	Joback Method

cpg	463.98	J/mol×K	804.60	Joback Method
cpg	473.56	J/mol×K	837.85	Joback Method
cpg	482.57	J/mol×K	871.10	Joback Method
cps	249.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0009312	Pa×s	424.77	Joback Method
dvisc	0.0004805	Pa×s	465.91	Joback Method
dvisc	0.0002760	Pa×s	507.04	Joback Method
dvisc	0.0001723	Pa×s	548.18	Joback Method
dvisc	0.0001149	Pa×s	589.32	Joback Method
dvisc	0.0000808	Pa×s	630.45	Joback Method
dvisc	0.0000593	Pa×s	671.59	Joback Method
hsubt	111.50 ± 1.70	kJ/mol	355.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.00164e+01
Coeff. B	-2.71791e+03
Coeff. C	-8.96020e+01
Temperature range (K), min.	368.97
Temperature range (K), max.	667.28

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243325&Units=SI

Legend

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume