2,3,6-Trimethylbenzoic acid

Inchi: InChI=1S/C10H12O2/c1-6-4-5-7(2)9(8(6)3)10(11)12/h4-5H,1-3H3,(H,11,12)
InchiKey: JRUKSSBDIZXQDX-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: Cc1ccc(C)c(C([O])=O)c1C
Mol. weight [g/mol]: 164.20
CAS: 2529-36-4

Physical Properties

Property code	Value	Unit	Source
chs	-5174.52 ± 0.84	kJ/mol	NIST Webbook
hf	-371.20 ± 1.90	kJ/mol	NIST Webbook
hfs	-475.60 ± 1.90	kJ/mol	NIST Webbook
hsub	104.40	kJ/mol	NIST Webbook
hsub	104.40 ± 0.20	kJ/mol	NIST Webbook
hsub	104.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-7.53		Crippen Method
logp	2.183		Crippen Method
mcvol	133.290	ml/mol	McGowan Method
rinpol	1402.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	103.60 ± 0.20	kJ/mol	325.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38828e+01

Coeff. B	-4.38457e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	411.00
Temperature range (K), max.	600.03

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2529364&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices