Benzoic acid, 2-(1-methylethyl)-

Inchi: InChI=1S/C10H12O2/c1-7(2)8-5-3-4-6-9(8)10(11)12/h3-7H,1-2H3,(H,11,12)
InchiKey: BANZVKGLDQDFDV-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)c1ccccc1C(=O)O
Mol. weight [g/mol]: 164.20
CAS: 2438-04-2

Physical Properties

Property code	Value	Unit	Source
chs	-5189.40 ± 1.30	kJ/mol	NIST Webbook
gf	-132.08	kJ/mol	Joback Method
hf	-359.20 ± 1.90	kJ/mol	NIST Webbook
hfs	-460.20 ± 1.90	kJ/mol	NIST Webbook
hfus	17.47	kJ/mol	Joback Method
hsub	101.00 ± 0.40	kJ/mol	NIST Webbook
hsub	101.00 ± 0.40	kJ/mol	NIST Webbook
hsub	101.00	kJ/mol	NIST Webbook
hvap	63.83	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.508		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	605.47	K	Joback Method
tc	810.65	K	Joback Method
tf	336.20 ± 1.50	K	NIST Webbook
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.64	J/mol×K	810.65	Joback Method
cpg	327.18	J/mol×K	605.47	Joback Method
cpg	338.54	J/mol×K	639.67	Joback Method
cpg	349.21	J/mol×K	673.86	Joback Method

cpg	359.23	J/mol×K	708.06	Joback Method
cpg	368.63	J/mol×K	742.25	Joback Method
cpg	377.42	J/mol×K	776.45	Joback Method
dvisc	0.0000831	Pa×s	605.47	Joback Method
dvisc	0.0058609	Pa×s	337.15	Joback Method
dvisc	0.0019034	Pa×s	381.87	Joback Method
dvisc	0.0007826	Pa×s	426.59	Joback Method
dvisc	0.0003809	Pa×s	471.31	Joback Method
dvisc	0.0002100	Pa×s	516.03	Joback Method
dvisc	0.0001273	Pa×s	560.75	Joback Method
hsubt	100.20 ± 0.40	kJ/mol	310.00	NIST Webbook

Sources

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=C2438042&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume