Benzoic acid, 3-(1-methylethyl)-

Inchi:	InChI=1S/C10H12O2/c1-7(2)8-4-3-5-9(6-8)10(11)12/h3-7H,1-2H3,(H,11,12)
InchiKey:	DLYVSJDCQZVKMD-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)c1cccc(C(=O)O)c1
Mol. weight [g/mol]:	164.20
CAS:	5651-47-8

Physical Properties

Property code	Value	Unit	Source
chs	-5170.10 ± 1.30	kJ/mol	NIST Webbook
gf	-132.08	kJ/mol	Joback Method
hf	-375.50 ± 1.90	kJ/mol	NIST Webbook
hfs	-479.60 ± 1.90	kJ/mol	NIST Webbook
hfus	17.47	kJ/mol	Joback Method
hsub	104.10 ± 0.30	kJ/mol	NIST Webbook
hsub	104.10 ± 0.30	kJ/mol	NIST Webbook
hsub	104.10	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	324.70 ± 2.00	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	103.30 ± 0.30	kJ/mol	308.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5651478&Units=SI
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

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

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