

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
mvol	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	m ³ /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	Paxs	605.47	Joback Method
dvisc	0.0058609	Paxs	337.15	Joback Method
dvisc	0.0019034	Paxs	381.87	Joback Method
dvisc	0.0007826	Paxs	426.59	Joback Method
dvisc	0.0003809	Paxs	471.31	Joback Method
dvisc	0.0002100	Paxs	516.03	Joback Method
dvisc	0.0001273	Paxs	560.75	Joback Method
hsubt	103.30 ± 0.30	kJ/mol	308.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5651478&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

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