

Benzoic acid, 2-formyl-

Other names:	2-Formylbenzoic acid 2-carboxybenzaldehyde 3-hydroxyphthalide Phthaldehydic acid o-Carboxybenzaldehyde o-Formylbenzoic acid o-Phthalaldehydic acid phthalaldehydic acid
Inchi:	InChI=1S/C8H6O3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-5H,(H,10,11)
InchiKey:	DYNFCHNNOHNJFG-UHFFFAOYSA-N
Formula:	C8H6O3
SMILES:	O=Cc1ccccc1C(=O)O
Mol. weight [g/mol]:	150.13
CAS:	119-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-246.00	kJ/mol	Joback Method
hf	-333.78	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.197		Crippen Method
mcvol	108.830	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	608.81	K	Joback Method
tc	864.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	371.61	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.78	J/molxK	608.81	Joback Method
cpg	281.48	J/molxK	784.01	Joback Method
cpg	275.53	J/molxK	748.97	Joback Method
cpg	269.11	J/molxK	713.93	Joback Method
cpg	262.19	J/molxK	678.89	Joback Method
cpg	254.76	J/molxK	643.85	Joback Method
cpg	286.98	J/molxK	819.05	Joback Method
dvisc	0.0001196	Paxs	608.81	Joback Method
dvisc	0.0001724	Paxs	569.28	Joback Method
dvisc	0.0002624	Paxs	529.74	Joback Method
dvisc	0.0004273	Paxs	490.21	Joback Method
dvisc	0.0007582	Paxs	450.68	Joback Method
dvisc	0.0015021	Paxs	411.14	Joback Method
dvisc	0.0034418	Paxs	371.61	Joback Method

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method:

<https://www.doi.org/10.1016/j.fluid.2014.07.038>

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=C119675&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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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