Benzoic acid, 3-formyl-

Other names: 3-Carboxybenzaldehyde
3-formylbenzoic acid
Inchi: InChI=1S/C8H6O3/c9-5-6-2-1-3-7(4-6)8(10)11/h1-5H,(H,10,11)
InchiKey: UHDNUPHSDMOGCR-UHFFFAOYSA-N
Formula: C8H6O3
SMILES: O=Cc1cccc(C(=O)O)c1
Mol. weight [g/mol]: 150.13
CAS: 619-21-6

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	819.05	K	Joback 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/mol×K	608.81	Joback Method
cpg	254.76	J/mol×K	643.85	Joback Method
cpg	262.19	J/mol×K	678.89	Joback Method
cpg	269.11	J/mol×K	713.93	Joback Method
cpg	275.53	J/mol×K	748.97	Joback Method
cpg	281.48	J/mol×K	784.01	Joback Method
cpg	286.98	J/mol×K	819.05	Joback Method

dvisc	0.0034418	Pa×s	371.61	Joback Method
dvisc	0.0015021	Pa×s	411.14	Joback Method
dvisc	0.0007582	Pa×s	450.68	Joback Method
dvisc	0.0004273	Pa×s	490.21	Joback Method
dvisc	0.0002624	Pa×s	529.74	Joback Method
dvisc	0.0001724	Pa×s	569.28	Joback Method
dvisc	0.0001196	Pa×s	608.81	Joback Method

Sources

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=C619216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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