p-Butyryloxybenzaldehyde

Other names: Butanoic acid, 4-formylphenyl ester
Inchi: InChI=1S/C11H12O3/c1-2-3-11(13)14-10-6-4-9(8-12)5-7-10/h4-8H,2-3H2,1H3
InchiKey: DAFTVVBQFUITOL-UHFFFAOYSA-N
Formula: C11H12O3
SMILES: CCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 192.21
CAS: 50262-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-188.92	kJ/mol	Joback Method
hf	-375.69	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.205		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	607.69	K	Joback Method
tc	820.81	K	Joback Method
tf	366.83	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.60	J/mol×K	607.69	Joback Method
cpg	376.20	J/mol×K	643.21	Joback Method
cpg	388.04	J/mol×K	678.73	Joback Method
cpg	399.15	J/mol×K	714.25	Joback Method
cpg	409.54	J/mol×K	749.77	Joback Method
cpg	419.22	J/mol×K	785.29	Joback Method
cpg	428.22	J/mol×K	820.81	Joback Method
dvisc	0.0017588	Pa×s	366.83	Joback Method

dvisc	0.0010582	Pa×s	406.97	Joback Method
dvisc	0.0006975	Pa×s	447.12	Joback Method
dvisc	0.0004925	Pa×s	487.26	Joback Method
dvisc	0.0003666	Pa×s	527.40	Joback Method
dvisc	0.0002846	Pa×s	567.55	Joback Method
dvisc	0.0002284	Pa×s	607.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.50 ± 1.50	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50262492&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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume