2-(Propionyloxy)benzoic acid

Inchi: InChI=1S/C10H10O4/c1-2-9(11)14-8-6-4-3-5-7(8)10(12)13/h3-6H,2H2,1H3,(H,12,13)
InchiKey: MDLKHAVFIDFTBO-UHFFFAOYSA-N
Formula: C10H10O4
SMILES: CCC(=O)Oc1ccccc1C(=O)O
Mol. weight [g/mol]: 194.18
CAS: 6328-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-363.56	kJ/mol	Joback Method
hf	-534.28	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.700		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	682.20	K	Joback Method
tc	888.42	K	Joback Method
tf	424.31	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.74	J/mol×K	682.20	Joback Method
cpg	404.35	J/mol×K	854.05	Joback Method
cpg	397.06	J/mol×K	819.68	Joback Method
cpg	389.16	J/mol×K	785.31	Joback Method
cpg	380.65	J/mol×K	750.94	Joback Method
cpg	371.51	J/mol×K	716.57	Joback Method
cpg	411.06	J/mol×K	888.42	Joback Method
dvisc	0.0000584	Pa×s	682.20	Joback Method
dvisc	0.0000831	Pa×s	639.22	Joback Method

dvisc	0.0001242	Pa×s	596.24	Joback Method
dvisc	0.0001977	Pa×s	553.25	Joback Method
dvisc	0.0003404	Pa×s	510.27	Joback Method
dvisc	0.0006477	Pa×s	467.29	Joback Method
dvisc	0.0014037	Pa×s	424.31	Joback Method

Sources

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=C6328445&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