Flopropione

Other names:	1-Propanone, 1-(2,4,6-trihydroxyphenyl)-
	Propiophenone, 2',4',6'-trihydroxy-
	Argobyl
	Cospanon
	Flopropion
	Labroda
	Labrodax
	Labrodax supanate
	Phloropropiophenone
	Propiophloroglucine
	RP 13907
	13907 R. P.
	2,4,6-Trihydroxypropiophenone
	2',4',6'-Trihydroxypropiophenone
	Chlonarin
	Ecapron
	Gasstenon
	Phloropropionone
	Supanate
	Supazlun
	Propionylphloroglucinol
	1-(2,4,6-Trihydroxyphenyl)-1-propanone
	Flopion
	Gallepronin
	Pasmus
	Profenon
	Spamorin
	Spasmoril
	NSC 97909
Inchi:	InChI=1S/C9H10O4/c1-2-6(11)9-7(12)3-5(10)4-8(9)13/h3-4,10,12-13H,2H2,1H3
InchiKey:	PTHLEKANMPKYDB-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	CCC(=O)c1c(O)cc(O)cc1O
Mol. weight [g/mol]:	182.17
CAS:	2295-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-455.47	kJ/mol	Joback Method
hf	-637.07	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	83.69	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.396		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	6493.16	kPa	Joback Method
tb	727.73	K	Joback Method
tc	975.37	K	Joback Method
tf	602.70	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.71	J/mol×K	727.73	Joback Method
cpg	371.32	J/mol×K	769.00	Joback Method
cpg	379.70	J/mol×K	810.28	Joback Method
cpg	388.07	J/mol×K	851.55	Joback Method
cpg	396.64	J/mol×K	892.83	Joback Method
cpg	405.64	J/mol×K	934.10	Joback Method
cpg	415.27	J/mol×K	975.37	Joback Method
dvisc	0.0000021	Pa×s	602.70	Joback Method
dvisc	0.0000013	Pa×s	623.54	Joback Method
dvisc	0.0000008	Pa×s	644.38	Joback Method
dvisc	0.0000005	Pa×s	665.22	Joback Method
dvisc	0.0000003	Pa×s	686.05	Joback Method
dvisc	0.0000002	Pa×s	706.89	Joback Method
dvisc	0.0000002	Pa×s	727.73	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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