Atranol

Other names: 2,6-Dihydroxy-4-methylbenzaldehyde
Inchi: InChI=1S/C8H8O3/c1-5-2-7(10)6(4-9)8(11)3-5/h2-4,10-11H,1H3
InchiKey: JASONGFGOLHLGB-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: Cc1cc(O)c(C=O)c(O)c1
Mol. weight [g/mol]: 152.15
CAS: 526-37-4

Physical Properties

Property code	Value	Unit	Source
gf	-289.50	kJ/mol	Joback Method
hf	-423.59	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.219		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5935.41	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1566.40		NIST Webbook
tb	624.00	K	Joback Method
tc	865.00	K	Joback Method
tf	484.30	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.44	J/mol×K	624.00	Joback Method
cpg	315.55	J/mol×K	824.83	Joback Method
cpg	308.78	J/mol×K	784.67	Joback Method
cpg	301.83	J/mol×K	744.50	Joback Method
cpg	294.54	J/mol×K	704.33	Joback Method

cpg	286.79	J/mol×K	664.17	Joback Method
cpg	322.25	J/mol×K	865.00	Joback Method
dvisc	0.0000064	Pa×s	624.00	Joback Method
dvisc	0.0000095	Pa×s	600.72	Joback Method
dvisc	0.0000144	Pa×s	577.43	Joback Method
dvisc	0.0000228	Pa×s	554.15	Joback Method
dvisc	0.0000374	Pa×s	530.87	Joback Method
dvisc	0.0000643	Pa×s	507.58	Joback Method
dvisc	0.0001164	Pa×s	484.30	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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C526374&Units=SI

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume