Ethyl 5-acetyl-2-hydroxybenzoate

Other names: 5-Acetyl-2-hydroxybenzoic acid, ethyl ester
Inchi: InChI=1S/C11H12O4/c1-3-15-11(14)9-6-8(7(2)12)4-5-10(9)13/h4-6,13H,3H2,1-2H3
InchiKey: VGKYNVLECUYQIL-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CCOC(=O)c1cc(C(C)=O)ccc1O
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	-372.94	kJ/mol	Joback Method
hf	-580.00	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.771		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	693.52	K	Joback Method
tc	920.09	K	Joback Method
tf	486.48	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.70	J/mol×K	693.52	Joback Method
cpg	459.65	J/mol×K	882.33	Joback Method
cpg	450.85	J/mol×K	844.56	Joback Method
cpg	441.52	J/mol×K	806.80	Joback Method
cpg	431.59	J/mol×K	769.04	Joback Method
cpg	421.00	J/mol×K	731.28	Joback Method
cpg	467.96	J/mol×K	920.09	Joback Method

dvisc	0.0000195	Pa×s	693.52	Joback Method
dvisc	0.0000273	Pa×s	659.01	Joback Method
dvisc	0.0000396	Pa×s	624.51	Joback Method
dvisc	0.0000602	Pa×s	590.00	Joback Method
dvisc	0.0000962	Pa×s	555.49	Joback Method
dvisc	0.0001636	Pa×s	520.99	Joback Method
dvisc	0.0003000	Pa×s	486.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373312&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/41-007-8/Ethyl-5-acetyl-2-hydroxybenzoate.pdf
Generated by Cheméo on 2024-04-19 00:39:00.450099063 +0000 UTC m=+15776389.370676378.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.