ethyl 4-methoxy-6-methylsalicylate

Other names: Ethyl 2-hydroxy-4-methoxy-6-methylbenzoate
Inchi: InChI=1S/C11H14O4/c1-4-15-11(13)10-7(2)5-8(14-3)6-9(10)12/h5-6,12H,4H2,1-3H3
InchiKey: PJOOIAZRUIIQMU-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCOC(=O)c1c(C)cc(OC)cc1O
Mol. weight [g/mol]: 210.23
CAS: 6110-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-358.65	kJ/mol	Joback Method
hf	-611.11	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.886		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1680.10		NIST Webbook
rinpol	1680.10		NIST Webbook
tb	667.05	K	Joback Method
tc	885.56	K	Joback Method
tf	471.30	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.53	J/mol×K	667.05	Joback Method
cpg	475.62	J/mol×K	849.14	Joback Method
cpg	465.83	J/mol×K	812.72	Joback Method
cpg	455.46	J/mol×K	776.31	Joback Method
cpg	444.47	J/mol×K	739.89	Joback Method
cpg	432.84	J/mol×K	703.47	Joback Method

cpg	484.86	J/mol×K	885.56	Joback Method
dvisc	0.0000170	Pa×s	667.05	Joback Method
dvisc	0.0000236	Pa×s	634.42	Joback Method
dvisc	0.0000340	Pa×s	601.80	Joback Method
dvisc	0.0000511	Pa×s	569.17	Joback Method
dvisc	0.0000807	Pa×s	536.55	Joback Method
dvisc	0.0001353	Pa×s	503.93	Joback Method
dvisc	0.0002436	Pa×s	471.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6110367&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

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