ethyl ferulate

Other names: Ferulic acid ethyl ester
ethyl 4'-hydroxy-3'-methoxycinnamate
Inchi: InChI=1S/C12H14O4/c1-3-16-12(14)7-5-9-4-6-10(13)11(8-9)15-2/h4-8,13H,3H2,1-2H3/b
InchiKey: ATJVZXXHKSYELS-FNORWQNLSA-N
Formula: C12H14O4
SMILES: CCOC(=O)C=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 222.24
CAS: 4046-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-260.38	kJ/mol	Joback Method
hf	-503.06	kJ/mol	Joback Method
hfus	30.45	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.977		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	689.11	K	Joback Method
tc	911.47	K	Joback Method
tf	464.97	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.01	J/mol×K	689.11	Joback Method
cpg	461.50	J/mol×K	726.17	Joback Method
cpg	473.24	J/mol×K	763.23	Joback Method
cpg	484.31	J/mol×K	800.29	Joback Method

cpg	494.75	J/mol×K	837.35	Joback Method
cpg	504.63	J/mol×K	874.41	Joback Method
cpg	514.01	J/mol×K	911.47	Joback Method
dvisc	0.0002591	Pa×s	464.97	Joback Method
dvisc	0.0001282	Pa×s	502.33	Joback Method
dvisc	0.0000699	Pa×s	539.68	Joback Method
dvisc	0.0000412	Pa×s	577.04	Joback Method
dvisc	0.0000259	Pa×s	614.40	Joback Method
dvisc	0.0000172	Pa×s	651.75	Joback Method
dvisc	0.0000119	Pa×s	689.11	Joback Method

Sources

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=C4046020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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