ethyl caffeate

Inchi: InChI=1S/C11H12O4/c1-2-15-11(14)6-4-8-3-5-9(12)10(13)7-8/h3-7,12-13H,2H2,1H3/b6-
InchiKey: WDKYDMULARNCIS-GQCTYLIASA-N
Formula: C11H12O4
SMILES: CCOC(=O)C=Cc1ccc(O)c(O)c1
Mol. weight [g/mol]: 208.21
CAS: 102-37-4

Physical Properties

Property code	Value	Unit	Source
gf	-308.79	kJ/mol	Joback Method
hf	-516.04	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	77.50	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.674		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	719.45	K	Joback Method
tc	955.96	K	Joback Method
tf	530.67	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.74	J/mol×K	719.45	Joback Method
cpg	431.38	J/mol×K	758.87	Joback Method
cpg	441.47	J/mol×K	798.29	Joback Method
cpg	451.17	J/mol×K	837.70	Joback Method
cpg	460.62	J/mol×K	877.12	Joback Method
cpg	469.97	J/mol×K	916.54	Joback Method
cpg	479.36	J/mol×K	955.96	Joback Method

dvisc	0.0000343	Pa×s	530.67	Joback Method
dvisc	0.0000168	Pa×s	562.13	Joback Method
dvisc	0.0000089	Pa×s	593.60	Joback Method
dvisc	0.0000050	Pa×s	625.06	Joback Method
dvisc	0.0000030	Pa×s	656.52	Joback Method
dvisc	0.0000019	Pa×s	687.99	Joback Method
dvisc	0.0000012	Pa×s	719.45	Joback Method

Sources

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=C102374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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