

Ethyl homovanillate

Other names:	Ethyl 4-hydroxy-3-methoxyphenyl acetate Benzeneacetic acid, 4-hydroxy-3-methoxy-, ethyl ester
Inchi:	InChI=1S/C11H14O4/c1-3-15-11(13)7-8-4-5-9(12)10(6-8)14-2/h4-6,12H,3,7H2,1-2H3
InchiKey:	AWPMWZHWVKXADV-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	CCOC(=O)Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	210.23
CAS:	60563-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-349.02	kJ/mol	Joback Method
hf	-599.64	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.506		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
ripol	2759.00		NIST Webbook
ripol	2759.00		NIST Webbook
ripol	2759.00		NIST Webbook
tb	662.07	K	Joback Method
tc	879.72	K	Joback Method
tf	458.78	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.72	J/mol×K	662.07	Joback Method
cpg	434.18	J/mol×K	698.34	Joback Method
cpg	445.92	J/mol×K	734.62	Joback Method
cpg	456.99	J/mol×K	770.89	Joback Method

cpg	467.41	J/mol×K	807.17	Joback Method
cpg	477.24	J/mol×K	843.44	Joback Method
cpg	486.51	J/mol×K	879.72	Joback Method
dvisc	0.0003177	Pa×s	458.78	Joback Method
dvisc	0.0001660	Pa×s	492.66	Joback Method
dvisc	0.0000943	Pa×s	526.54	Joback Method
dvisc	0.0000573	Pa×s	560.42	Joback Method
dvisc	0.0000369	Pa×s	594.31	Joback Method
dvisc	0.0000249	Pa×s	628.19	Joback Method
dvisc	0.0000175	Pa×s	662.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60563135&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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