ETHYL 2,4-DIHYDROXY-6-METHYLBENZOATE

Other names:	«beta»-Resorcylic acid, 6-methyl-, ethyl ester
	o-Orsellinic acid, ethyl ester
	Benzoic acid, 2,4-dihydroxy-6-methyl-, ethyl ester
	Ethyl orsellinate
	Orsellinic acid, ethyl ester
Inchi:	InChI=1S/C10H12O4/c1-3-14-10(13)9-6(2)4-7(11)5-8(9)12/h4-5,11-12H,3H2,1-2H3
InchiKey:	UQSRXQMIXSZGLA-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	CCOC(=O)c1c(C)cc(O)cc1O
Mol. weight [g/mol]:	196.20

Physical Properties

Property code	Value	Unit	Source
af	0.7854		Cheméo Relay (1.0)
hf	-689.00	kJ/mol	Cheméo Relay (1.0)
hfus	29.66	kJ/mol	Joback Method
hvap	95.49	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-2.85		Cheméo Relay (1.0)
logp	1.583		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
rinpol	1758.70		NIST Webbook
tb	574.00	K	Cheméo Relay (1.0)
tc	815.24	K	Cheméo Relay (1.0)
tf	390.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.47	J/mol×K	697.39	Joback Method
cpg	403.91	J/mol×K	736.19	Joback Method
cpg	413.81	J/mol×K	774.99	Joback Method
cpg	423.27	J/mol×K	813.79	Joback Method

cpg	432.40	J/mol×K	852.59	Joback Method
cpg	441.31	J/mol×K	891.39	Joback Method
cpg	450.12	J/mol×K	930.19	Joback Method
dvisc	0.0000324	Pa×s	537.00	Joback Method
dvisc	0.0000180	Pa×s	563.73	Joback Method
dvisc	0.0000106	Pa×s	590.46	Joback Method
dvisc	0.0000065	Pa×s	617.19	Joback Method
dvisc	0.0000042	Pa×s	643.93	Joback Method
dvisc	0.0000028	Pa×s	670.66	Joback Method
dvisc	0.0000019	Pa×s	697.39	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2524370&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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