

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
CAS:	2524-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-407.06	kJ/mol	Joback Method
hf	-624.09	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	75.98	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.583		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
rinpol	1758.70		NIST Webbook
tb	697.39	K	Joback Method
tc	930.19	K	Joback Method
tf	537.00	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.47	J/mol×K	697.39	Joback Method
cpg	441.31	J/mol×K	891.39	Joback Method
cpg	432.40	J/mol×K	852.59	Joback Method

cpg	423.27	J/mol×K	813.79	Joback Method
cpg	413.81	J/mol×K	774.99	Joback Method
cpg	403.91	J/mol×K	736.19	Joback Method
cpg	450.12	J/mol×K	930.19	Joback Method
dvisc	0.0000019	Pa×s	697.39	Joback Method
dvisc	0.0000028	Pa×s	670.66	Joback Method
dvisc	0.0000042	Pa×s	643.93	Joback Method
dvisc	0.0000065	Pa×s	617.19	Joback Method
dvisc	0.0000106	Pa×s	590.46	Joback Method
dvisc	0.0000180	Pa×s	563.73	Joback Method
dvisc	0.0000324	Pa×s	537.00	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=C2524370&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

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