

ethyl 2,4-dihydroxy-3,6-dimethylbenzoate

Inchi:	InChI=1S/C11H14O4/c1-4-15-11(14)9-6(2)5-8(12)7(3)10(9)13/h5,12-13H,4H2,1-3H3
InchiKey:	VJLLNFDLMWPNBN-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	CCOC(=O)c1c(C)cc(O)c(C)c1O
Mol. weight [g/mol]:	210.23
CAS:	31581-32-5

Physical Properties

Property code	Value	Unit	Source
gf	-408.27	kJ/mol	Joback Method
hf	-656.20	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.891		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1796.70		NIST Webbook
tb	725.25	K	Joback Method
tc	954.55	K	Joback Method
tf	560.79	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.87	J/mol×K	725.25	Joback Method
cpg	453.01	J/mol×K	763.47	Joback Method
cpg	463.65	J/mol×K	801.68	Joback Method
cpg	473.88	J/mol×K	839.90	Joback Method
cpg	483.81	J/mol×K	878.12	Joback Method
cpg	493.53	J/mol×K	916.33	Joback Method
cpg	503.15	J/mol×K	954.55	Joback Method
dvisc	0.0000200	Pa×s	560.79	Joback Method

dvisc	0.0000115	Pa×s	588.20	Joback Method
dvisc	0.0000069	Pa×s	615.61	Joback Method
dvisc	0.0000044	Pa×s	643.02	Joback Method
dvisc	0.0000029	Pa×s	670.43	Joback Method
dvisc	0.0000019	Pa×s	697.84	Joback Method
dvisc	0.0000013	Pa×s	725.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31581325&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
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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