

Isopropyl 3-formyl-2,4-dihydroxy-6-methylbenzoate

Inchi:	InChI=1S/C12H14O5/c1-6(2)17-12(16)10-7(3)4-9(14)8(5-13)11(10)15/h4-6,14-15H,1-3H
InchiKey:	BECXOCBQWLOZFB-UHFFFAOYSA-N
Formula:	C12H14O5
SMILES:	<chem>Cc1cc(O)c(C=O)c(O)c1C(=O)OC(C)C</chem>
Mol. weight [g/mol]:	238.24
CAS:	1245608-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-501.81	kJ/mol	Joback Method
hf	-767.70	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.784		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	796.35	K	Joback Method
tc	1026.97	K	Joback Method
tf	599.06	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.65	J/molxK	796.35	Joback Method
cpg	514.43	J/molxK	834.79	Joback Method
cpg	524.81	J/molxK	873.22	Joback Method
cpg	534.89	J/molxK	911.66	Joback Method
cpg	544.77	J/molxK	950.10	Joback Method
cpg	554.57	J/molxK	988.54	Joback Method
cpg	564.38	J/molxK	1026.97	Joback Method
dvisc	0.0000131	Paxs	599.06	Joback Method
dvisc	0.0000072	Paxs	631.94	Joback Method

dvisc	0.0000041	Paxs	664.82	Joback Method
dvisc	0.0000025	Paxs	697.71	Joback Method
dvisc	0.0000016	Paxs	730.59	Joback Method
dvisc	0.0000011	Paxs	763.47	Joback Method
dvisc	0.0000007	Paxs	796.35	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=C1245608154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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