Propyl 2,4-dihydroxy-6-methylbenzoate

Inchi: InChI=1S/C11H14O4/c1-3-4-15-11(14)10-7(2)5-8(12)6-9(10)13/h5-6,12-13H,3-4H2,1-2H
InchiKey: WHFPMVZTSUOBEX-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCCOC(=O)c1c(C)cc(O)cc1O
Mol. weight [g/mol]: 210.23
CAS: 31581-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-398.64	kJ/mol	Joback Method
hf	-644.73	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	78.20	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.973		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	1786.20		NIST Webbook
rinpol	1786.20		NIST Webbook
tb	720.27	K	Joback Method
tc	948.77	K	Joback Method
tf	548.27	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.44	J/mol×K	720.27	Joback Method
cpg	495.18	J/mol×K	910.69	Joback Method
cpg	485.49	J/mol×K	872.61	Joback Method
cpg	475.58	J/mol×K	834.52	Joback Method
cpg	465.34	J/mol×K	796.44	Joback Method
cpg	454.66	J/mol×K	758.35	Joback Method
cpg	504.75	J/mol×K	948.77	Joback Method

dvisc	0.0000014	Pa×s	720.27	Joback Method
dvisc	0.0000021	Pa×s	691.60	Joback Method
dvisc	0.0000031	Pa×s	662.94	Joback Method
dvisc	0.0000050	Pa×s	634.27	Joback Method
dvisc	0.0000082	Pa×s	605.60	Joback Method
dvisc	0.0000143	Pa×s	576.94	Joback Method
dvisc	0.0000262	Pa×s	548.27	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=C31581290&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