3H-2-Benzopyran-7-carboxylic acid, 4,6-dihydro-8-hydroxy-3,4,5-trimethyl-6-oxo-, (3S-trans)-

InChI: InChI=1S/C12H12O5/c1-5-6(2)17-4-8-7(5)3-9(13)10(11(8)14)12(15)16/h3-6,14H,1-2H3,(

InChIKey: UKOIKDGZQBFMQS-PHDIDXHHSA-N

Formula: C13H14O5

SMILES: CC1OC=C2C(=CC(=O)C(C(=O)O)=C2O)C1C

Mol. weight [g/mol]: 250.25

CAS: 112245-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-436.65	kJ/mol	Joback Method
hf	-729.33	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	95.20	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.331		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	854.92	K	Joback Method
tc	1069.44	K	Joback Method
tf	565.52	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.41	J/mol×K	854.92	Joback Method
cpg	519.96	J/mol×K	890.67	Joback Method
cpg	528.67	J/mol×K	926.43	Joback Method
cpg	536.54	J/mol×K	962.18	Joback Method
cpg	543.58	J/mol×K	997.93	Joback Method
cpg	549.79	J/mol×K	1033.69	Joback Method
cpg	555.17	J/mol×K	1069.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112245940&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

Legend

cpg:	Ideal gas heat capacity
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