1-Propanone, 3-hydroxy-1,3,3-triphenyl-

Inchi: InChI=1S/C21H18O2/c22-20(17-10-4-1-5-11-17)16-21(23,18-12-6-2-7-13-18)19-14-8-3-9
InchiKey: NWFJIBVQGLMVTB-UHFFFAOYSA-N
Formula: C21H18O2
SMILES: O=C(CC(O)(c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 302.37
CAS: 6624-02-8

Physical Properties

Property code	Value	Unit	Source
chs	-10600.00	kJ/mol	NIST Webbook
gf	200.27	kJ/mol	Joback Method
hf	-40.74	kJ/mol	Joback Method
hfs	-240.80	kJ/mol	NIST Webbook
hfus	30.54	kJ/mol	Joback Method
hvap	91.30	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.196		Crippen Method
mcvol	242.910	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	902.74	K	Joback Method
tc	1150.28	K	Joback Method
tf	518.86	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.89	J/mol×K	902.74	Joback Method
cpg	783.07	J/mol×K	1109.02	Joback Method
cpg	773.41	J/mol×K	1067.77	Joback Method
cpg	763.22	J/mol×K	1026.51	Joback Method
cpg	752.35	J/mol×K	985.25	Joback Method
cpg	740.62	J/mol×K	944.00	Joback Method
cpg	792.38	J/mol×K	1150.28	Joback Method

dvisc	0.0000102	Pa×s	902.74	Joback Method
dvisc	0.0000150	Pa×s	838.76	Joback Method
dvisc	0.0000236	Pa×s	774.78	Joback Method
dvisc	0.0000403	Pa×s	710.80	Joback Method
dvisc	0.0000763	Pa×s	646.82	Joback Method
dvisc	0.0001665	Pa×s	582.84	Joback Method
dvisc	0.0004401	Pa×s	518.86	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=C6624028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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