Tetra-t-amylperoxypyromellitate

Inchi: InChI=1S/C30H46O12/c1-13-27(5,6)39-35-23(31)19-17-21(25(33)37-41-29(9,10)15-3)22
InchiKey: BMLIINUSXIWIJB-UHFFFAOYSA-N
Formula: C30H46O12
SMILES: CCC(C)(C)OOC(=O)c1cc(C(=O)OOC(C)(C)CC)c(C(=O)OOC(C)(C)CC)cc1C(=O)OOC(C
Mol. weight [g/mol]: 598.68
CAS: 77473-07-5

Physical Properties

Property code	Value	Unit	Source
chs	-16617.60 ± 6.30	kJ/mol	NIST Webbook
gf	-1059.08	kJ/mol	Joback Method
hf	-2003.49	kJ/mol	Joback Method
hfs	-1761.90 ± 6.70	kJ/mol	NIST Webbook
hfus	52.57	kJ/mol	Joback Method
hvap	127.72	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	6.795		Crippen Method
mcvol	463.040	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
tb	1309.34	K	Joback Method
tc	1647.85	K	Joback Method
tf	879.08	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1623.09	J/mol×K	1309.34	Joback Method
cpg	1620.86	J/mol×K	1365.76	Joback Method
cpg	1614.09	J/mol×K	1422.18	Joback Method
cpg	1602.90	J/mol×K	1478.59	Joback Method
cpg	1587.40	J/mol×K	1535.01	Joback Method
cpg	1567.71	J/mol×K	1591.43	Joback Method
cpg	1543.96	J/mol×K	1647.85	Joback Method

dvisc	0.0000038	Pa×s	879.08	Joback Method
dvisc	0.0000023	Pa×s	950.79	Joback Method
dvisc	0.0000015	Pa×s	1022.50	Joback Method
dvisc	0.0000010	Pa×s	1094.21	Joback Method
dvisc	0.0000007	Pa×s	1165.92	Joback Method
dvisc	0.0000005	Pa×s	1237.63	Joback Method
dvisc	0.0000004	Pa×s	1309.34	Joback Method

Sources

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=C77473075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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