Tetra-t-butylperoxypyromellitate

Inchi: InChI=1S/C26H38O12/c1-23(2,3)35-31-19(27)15-13-17(21(29)33-37-25(7,8)9)18(22(30)
InchiKey: KOAKWBXPXOTXGD-UHFFFAOYSA-N
Formula: C26H38O12
SMILES: CC(C)(C)OOC(=O)c1cc(C(=O)OOC(C)(C)C)c(C(=O)OOC(C)(C)C)cc1C(=O)OOC(C)(C)C
Mol. weight [g/mol]: 542.57
CAS: 63472-69-5

Physical Properties

Property code	Value	Unit	Source
chs	-14126.60 ± 7.60	kJ/mol	NIST Webbook
gf	-1092.76	kJ/mol	Joback Method
hf	-1920.93	kJ/mol	Joback Method
hfs	-1536.10 ± 7.60	kJ/mol	NIST Webbook
hfus	42.21	kJ/mol	Joback Method
hvap	118.81	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	5.234		Crippen Method
mcvol	406.680	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
tb	1217.82	K	Joback Method
tc	1500.88	K	Joback Method
tf	834.00	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.36	J/mol×K	1217.82	Joback Method
cpg	1396.37	J/mol×K	1265.00	Joback Method
cpg	1395.22	J/mol×K	1312.17	Joback Method
cpg	1390.96	J/mol×K	1359.35	Joback Method
cpg	1383.61	J/mol×K	1406.53	Joback Method
cpg	1373.22	J/mol×K	1453.70	Joback Method
cpg	1359.83	J/mol×K	1500.88	Joback Method

dvisc	0.0000069	Pa×s	834.00	Joback Method
dvisc	0.0000043	Pa×s	897.97	Joback Method
dvisc	0.0000029	Pa×s	961.94	Joback Method
dvisc	0.0000020	Pa×s	1025.91	Joback Method
dvisc	0.0000014	Pa×s	1089.88	Joback Method
dvisc	0.0000011	Pa×s	1153.85	Joback Method
dvisc	0.0000008	Pa×s	1217.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63472695&Units=SI

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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