1,4-Di-t-butylperoxy pyromellitate

Inchi: InChI=1S/C18H22O10/c1-17(2,3)27-25-15(23)11-7-10(14(21)22)12(8-9(11)13(19)20)16(
InchiKey: MXFZJFCNTQTGHU-UHFFFAOYSA-N
Formula: C18H22O10
SMILES: CC(C)(C)OOC(=O)c1cc(C(=O)O)c(C(=O)OOC(C)(C)C)cc1C(=O)O
Mol. weight [g/mol]: 398.36
CAS: 82234-37-5

Physical Properties

Property code	Value	Unit	Source
chs	-8566.10 ± 6.00	kJ/mol	NIST Webbook
gf	-1019.44	kJ/mol	Joback Method
hf	-1513.89	kJ/mol	Joback Method
hfs	-1661.80 ± 6.00	kJ/mol	NIST Webbook
hfus	39.75	kJ/mol	Joback Method
hvap	127.31	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	2.857		Crippen Method
mcvol	282.220	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
tb	1135.92	K	Joback Method
tc	1396.14	K	Joback Method
tf	771.72	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.47	J/mol×K	1135.92	Joback Method
cpg	921.08	J/mol×K	1179.29	Joback Method
cpg	923.99	J/mol×K	1222.66	Joback Method
cpg	925.22	J/mol×K	1266.03	Joback Method
cpg	924.82	J/mol×K	1309.40	Joback Method
cpg	922.80	J/mol×K	1352.77	Joback Method
cpg	919.21	J/mol×K	1396.14	Joback Method

dvisc	0.0000046	Pa×s	771.72	Joback Method
dvisc	0.0000023	Pa×s	832.42	Joback Method
dvisc	0.0000013	Pa×s	893.12	Joback Method
dvisc	0.0000008	Pa×s	953.82	Joback Method
dvisc	0.0000005	Pa×s	1014.52	Joback Method
dvisc	0.0000003	Pa×s	1075.22	Joback Method
dvisc	0.0000002	Pa×s	1135.92	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=C82234375&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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