Di-t-amylperoxypyromellitate

Inchi: InChI=1S/C20H26O10/c1-7-19(3,4)29-27-17(25)13-9-12(16(23)24)14(10-11(13)15(21)22
InchiKey: YJTOFETZPVDRDI-UHFFFAOYSA-N
Formula: C20H26O10
SMILES: CCC(C)(C)OOC(=O)c1cc(C(=O)O)c(C(=O)OOC(C)(C)CC)cc1C(=O)O
Mol. weight [g/mol]: 426.41
CAS: 77494-58-7

Physical Properties

Property code	Value	Unit	Source
chs	-9945.40 ± 6.00	kJ/mol	NIST Webbook
gf	-1002.60	kJ/mol	Joback Method
hf	-1555.17	kJ/mol	Joback Method
hfs	-1640.60 ± 6.10	kJ/mol	NIST Webbook
hfus	44.93	kJ/mol	Joback Method
hvap	131.77	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	3.637		Crippen Method
mcvol	310.400	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
tb	1181.68	K	Joback Method
tc	1462.63	K	Joback Method
tf	794.26	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.33	J/mol×K	1181.68	Joback Method
cpg	1035.77	J/mol×K	1228.51	Joback Method
cpg	1038.18	J/mol×K	1275.33	Joback Method
cpg	1038.60	J/mol×K	1322.16	Joback Method
cpg	1037.09	J/mol×K	1368.98	Joback Method
cpg	1033.70	J/mol×K	1415.81	Joback Method
cpg	1028.49	J/mol×K	1462.63	Joback Method

dvisc	0.0000032	Pa×s	794.26	Joback Method
dvisc	0.0000016	Pa×s	858.83	Joback Method
dvisc	0.0000009	Pa×s	923.40	Joback Method
dvisc	0.0000005	Pa×s	987.97	Joback Method
dvisc	0.0000003	Pa×s	1052.54	Joback Method
dvisc	0.0000002	Pa×s	1117.11	Joback Method
dvisc	0.0000001	Pa×s	1181.68	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=C77494587&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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