Dimethyl pyromellitate

Inchi: InChI=1S/C12H10O8/c1-19-11(17)7-3-6(10(15)16)8(12(18)20-2)4-5(7)9(13)14/h3-4H,1-2
InchiKey: QUNAYECDJMFUKV-UHFFFAOYSA-N
Formula: C12H10O8
SMILES: COC(=O)c1cc(C(=O)O)c(C(=O)OC)cc1C(=O)O
Mol. weight [g/mol]: 282.20
CAS: 39900-53-3

Physical Properties

Property code	Value	Unit	Source
chs	-4672.70 ± 2.60	kJ/mol	NIST Webbook
gf	-865.64	kJ/mol	Joback Method
hf	-1108.11	kJ/mol	Joback Method
hfs	-1478.60 ± 2.60	kJ/mol	NIST Webbook
hfus	36.66	kJ/mol	Joback Method
hvap	111.73	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	0.656		Crippen Method
mcvol	185.940	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	960.26	K	Joback Method
tc	1178.80	K	Joback Method
tf	654.80	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.13	J/mol×K	960.26	Joback Method
cpg	540.73	J/mol×K	996.68	Joback Method
cpg	545.39	J/mol×K	1033.11	Joback Method
cpg	549.10	J/mol×K	1069.53	Joback Method
cpg	551.85	J/mol×K	1105.95	Joback Method
cpg	553.61	J/mol×K	1142.38	Joback Method
cpg	554.39	J/mol×K	1178.80	Joback Method

dvisc	0.0000505	Pa×s	654.80	Joback Method
dvisc	0.0000261	Pa×s	705.71	Joback Method
dvisc	0.0000147	Pa×s	756.62	Joback Method
dvisc	0.0000089	Pa×s	807.53	Joback Method
dvisc	0.0000058	Pa×s	858.44	Joback Method
dvisc	0.0000039	Pa×s	909.35	Joback Method
dvisc	0.0000028	Pa×s	960.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39900533&Units=SI
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

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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