Pimelic acid, di(4-formylphenyl) ester

Inchi: InChI=1S/C21H20O6/c22-14-16-6-10-18(11-7-16)26-20(24)4-2-1-3-5-21(25)27-19-12-8-1
InchiKey: DQAMRWBFIWELFN-UHFFFAOYSA-N
Formula: C21H20O6
SMILES: O=Cc1ccc(OC(=O)CCCCCC(=O)Oc2ccc(C=O)cc2)cc1
Mol. weight [g/mol]: 368.38

Physical Properties

Property code	Value	Unit	Source
gf	-335.38	kJ/mol	Joback Method
hf	-687.41	kJ/mol	Joback Method
hfus	47.60	kJ/mol	Joback Method
hvap	99.97	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.773		Crippen Method
mcvol	277.250	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2268.00		NIST Webbook
tb	993.10	K	Joback Method
tc	1225.39	K	Joback Method
tf	632.63	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.35	J/mol×K	993.10	Joback Method
cpg	864.20	J/mol×K	1031.81	Joback Method
cpg	872.74	J/mol×K	1070.53	Joback Method
cpg	880.00	J/mol×K	1109.24	Joback Method
cpg	886.02	J/mol×K	1147.96	Joback Method
cpg	890.83	J/mol×K	1186.67	Joback Method
cpg	894.48	J/mol×K	1225.39	Joback Method
dvisc	0.0004014	Pa×s	632.63	Joback Method
dvisc	0.0002527	Pa×s	692.71	Joback Method

dvisc	0.0001713	Pa×s	752.79	Joback Method
dvisc	0.0001230	Pa×s	812.87	Joback Method
dvisc	0.0000924	Pa×s	872.94	Joback Method
dvisc	0.0000721	Pa×s	933.02	Joback Method
dvisc	0.0000579	Pa×s	993.10	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=U416652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume