Pimelic acid, 4-formylphenyl pentyl ester

Inchi: InChI=1S/C19H26O5/c1-2-3-7-14-23-18(21)8-5-4-6-9-19(22)24-17-12-10-16(15-20)11-13
InchiKey: NBDXCBLWLJLSAF-UHFFFAOYSA-N
Formula: C19H26O5
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-355.48	kJ/mol	Joback Method
hf	-785.61	kJ/mol	Joback Method
hfus	46.48	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.088		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
tb	867.02	K	Joback Method
tc	1071.96	K	Joback Method
tf	529.15	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.14	J/mol×K	867.02	Joback Method
cpg	849.23	J/mol×K	901.18	Joback Method
cpg	862.21	J/mol×K	935.33	Joback Method
cpg	874.10	J/mol×K	969.49	Joback Method
cpg	884.91	J/mol×K	1003.65	Joback Method
cpg	894.68	J/mol×K	1037.81	Joback Method
cpg	903.43	J/mol×K	1071.96	Joback Method
dvisc	0.0006244	Pa×s	529.15	Joback Method

dvisc	0.0003612	Pa×s	585.46	Joback Method
dvisc	0.0002301	Pa×s	641.77	Joback Method
dvisc	0.0001576	Pa×s	698.09	Joback Method
dvisc	0.0001142	Pa×s	754.40	Joback Method
dvisc	0.0000865	Pa×s	810.71	Joback Method
dvisc	0.0000680	Pa×s	867.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416647&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

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