Pimelic acid, 4-formylphenyl octyl ester

Inchi: InChI=1S/C22H32O5/c1-2-3-4-5-6-10-17-26-21(24)11-8-7-9-12-22(25)27-20-15-13-19(18
InchiKey: RWNCPPSDPRBUEP-UHFFFAOYSA-N
Formula: C22H32O5
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-330.22	kJ/mol	Joback Method
hf	-847.53	kJ/mol	Joback Method
hfus	54.25	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.259		Crippen Method
mcvol	313.530	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	3006.00		NIST Webbook
rinpol	3006.00		NIST Webbook
tb	935.66	K	Joback Method
tc	1147.01	K	Joback Method
tf	562.96	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.63	J/mol×K	935.66	Joback Method
cpg	1073.81	J/mol×K	1111.79	Joback Method
cpg	1064.02	J/mol×K	1076.56	Joback Method
cpg	1053.03	J/mol×K	1041.34	Joback Method
cpg	1040.83	J/mol×K	1006.11	Joback Method
cpg	1027.37	J/mol×K	970.89	Joback Method
cpg	1082.45	J/mol×K	1147.01	Joback Method
dvisc	0.0000442	Pa×s	935.66	Joback Method

dvisc	0.0000567	Pa×s	873.54	Joback Method
dvisc	0.0000757	Pa×s	811.43	Joback Method
dvisc	0.0001060	Pa×s	749.31	Joback Method
dvisc	0.0001577	Pa×s	687.19	Joback Method
dvisc	0.0002539	Pa×s	625.08	Joback Method
dvisc	0.0004541	Pa×s	562.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416650&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

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