Pimelic acid, ethyl 4-formylphenyl ester

Inchi: InChI=1S/C16H20O5/c1-2-20-15(18)6-4-3-5-7-16(19)21-14-10-8-13(12-17)9-11-14/h8-12
InchiKey: DLPXPVZDYMRSNX-UHFFFAOYSA-N
Formula: C16H20O5
SMILES: CCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-380.74	kJ/mol	Joback Method
hf	-723.69	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.918		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	798.38	K	Joback Method
tc	1003.67	K	Joback Method
tf	495.34	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.44	J/mol×K	798.38	Joback Method
cpg	721.37	J/mol×K	969.45	Joback Method
cpg	711.90	J/mol×K	935.24	Joback Method
cpg	701.48	J/mol×K	901.02	Joback Method
cpg	690.11	J/mol×K	866.81	Joback Method
cpg	677.76	J/mol×K	832.59	Joback Method
cpg	729.91	J/mol×K	1003.67	Joback Method
dvisc	0.0001022	Pa×s	798.38	Joback Method

dvisc	0.0001287	Pa×s	747.87	Joback Method
dvisc	0.0001676	Pa×s	697.37	Joback Method
dvisc	0.0002275	Pa×s	646.86	Joback Method
dvisc	0.0003252	Pa×s	596.35	Joback Method
dvisc	0.0004966	Pa×s	545.85	Joback Method
dvisc	0.0008267	Pa×s	495.34	Joback Method

Sources

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=U416642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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