Pimelic acid, 4-formylphenyl propyl ester

Inchi: InChI=1S/C17H22O5/c1-2-12-21-16(19)6-4-3-5-7-17(20)22-15-10-8-14(13-18)9-11-15/h8
InchiKey: ZAFFGGRYMPLDKV-UHFFFAOYSA-N
Formula: C17H22O5
SMILES: CCCOC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-372.32	kJ/mol	Joback Method
hf	-744.33	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.308		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	821.26	K	Joback Method
tc	1025.77	K	Joback Method
tf	506.61	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.47	J/mol×K	821.26	Joback Method
cpg	778.43	J/mol×K	991.69	Joback Method
cpg	768.82	J/mol×K	957.60	Joback Method
cpg	758.24	J/mol×K	923.52	Joback Method
cpg	746.66	J/mol×K	889.43	Joback Method
cpg	734.08	J/mol×K	855.35	Joback Method
cpg	787.07	J/mol×K	1025.77	Joback Method
dvisc	0.0000895	Pa×s	821.26	Joback Method

dvisc	0.0001131	Pa×s	768.82	Joback Method
dvisc	0.0001480	Pa×s	716.38	Joback Method
dvisc	0.0002020	Pa×s	663.93	Joback Method
dvisc	0.0002909	Pa×s	611.49	Joback Method
dvisc	0.0004485	Pa×s	559.05	Joback Method
dvisc	0.0007564	Pa×s	506.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416643&Units=SI

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