Pimelic acid, 4-formylphenyl isobutyl ester

Inchi: InChI=1S/C18H24O5/c1-14(2)13-22-17(20)6-4-3-5-7-18(21)23-16-10-8-15(12-19)9-11-16
InchiKey: OGVZITLXRYJPSO-UHFFFAOYSA-N
Formula: C18H24O5
SMILES: CC(C)COC(=O)CCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-366.34	kJ/mol	Joback Method
hf	-770.25	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.554		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	843.70	K	Joback Method
tc	1050.11	K	Joback Method
tf	502.88	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.94	J/mol×K	843.70	Joback Method
cpg	791.92	J/mol×K	878.10	Joback Method
cpg	804.81	J/mol×K	912.50	Joback Method
cpg	816.61	J/mol×K	946.90	Joback Method
cpg	827.36	J/mol×K	981.30	Joback Method
cpg	837.06	J/mol×K	1015.70	Joback Method
cpg	845.73	J/mol×K	1050.11	Joback Method
dvisc	0.0007683	Pa×s	502.88	Joback Method

dvisc	0.0004232	Pa×s	559.68	Joback Method
dvisc	0.0002602	Pa×s	616.49	Joback Method
dvisc	0.0001737	Pa×s	673.29	Joback Method
dvisc	0.0001234	Pa×s	730.09	Joback Method
dvisc	0.0000922	Pa×s	786.90	Joback Method
dvisc	0.0000716	Pa×s	843.70	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=U416644&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