Pimelic acid, butyl 4-formylphenyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-363.90	kJ/mol	Joback Method
hf	-764.97	kJ/mol	Joback Method
hfus	43.89	kJ/mol	Joback Method
hvap	83.63	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.698		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	844.14	K	Joback Method
tc	1048.52	K	Joback Method
tf	517.88	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.40	J/mol×K	844.14	Joback Method
cpg	836.21	J/mol×K	1014.46	Joback Method
cpg	826.51	J/mol×K	980.39	Joback Method
cpg	815.79	J/mol×K	946.33	Joback Method
cpg	804.05	J/mol×K	912.27	Joback Method
cpg	791.25	J/mol×K	878.20	Joback Method
cpg	844.92	J/mol×K	1048.52	Joback Method
dvisc	0.0000781	Pa×s	844.14	Joback Method

dvisc	0.0000991	Pa×s	789.76	Joback Method
dvisc	0.0001302	Pa×s	735.39	Joback Method
dvisc	0.0001787	Pa×s	681.01	Joback Method
dvisc	0.0002592	Pa×s	626.63	Joback Method
dvisc	0.0004034	Pa×s	572.26	Joback Method
dvisc	0.0006888	Pa×s	517.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416645&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