Isophthalic acid, 4-formylphenyl isohexyl ester

Inchi: InChI=1S/C21H22O5/c1-15(2)5-4-12-25-20(23)17-6-3-7-18(13-17)21(24)26-19-10-8-16(1
InchiKey: SVOANPXFGNXLRQ-UHFFFAOYSA-N
Formula: C21H22O5
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc(C=O)cc2)c1
Mol. weight [g/mol]: 354.40

Physical Properties

Property code	Value	Unit	Source
gf	-238.30	kJ/mol	Joback Method
hf	-607.11	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	92.86	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.311		Crippen Method
mcvol	275.680	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	944.00	K	Joback Method
tc	1173.39	K	Joback Method
tf	575.63	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.76	J/mol×K	944.00	Joback Method
cpg	860.82	J/mol×K	982.23	Joback Method
cpg	871.53	J/mol×K	1020.46	Joback Method
cpg	880.94	J/mol×K	1058.69	Joback Method
cpg	889.07	J/mol×K	1096.93	Joback Method
cpg	895.97	J/mol×K	1135.16	Joback Method
cpg	901.66	J/mol×K	1173.39	Joback Method
dvisc	0.0004350	Pa×s	575.63	Joback Method

dvisc	0.0002537	Pa×s	637.02	Joback Method
dvisc	0.0001627	Pa×s	698.42	Joback Method
dvisc	0.0001121	Pa×s	759.82	Joback Method
dvisc	0.0000817	Pa×s	821.21	Joback Method
dvisc	0.0000622	Pa×s	882.61	Joback Method
dvisc	0.0000491	Pa×s	944.00	Joback Method

Sources

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=U344694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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