Isophthalic acid, 4-formylphenyl hexyl ester

Inchi: InChI=1S/C21H22O5/c1-2-3-4-5-13-25-20(23)17-7-6-8-18(14-17)21(24)26-19-11-9-16(15
InchiKey: RAHJVMVBTGGAGP-UHFFFAOYSA-N
Formula: C21H22O5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C=O)cc2)c1
Mol. weight [g/mol]: 354.40

Physical Properties

Property code	Value	Unit	Source
gf	-235.86	kJ/mol	Joback Method
hf	-601.83	kJ/mol	Joback Method
hfus	45.31	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.455		Crippen Method
mcvol	275.680	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	944.44	K	Joback Method
tc	1171.66	K	Joback Method
tf	590.63	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.27	J/mol×K	944.44	Joback Method
cpg	860.27	J/mol×K	982.31	Joback Method
cpg	870.96	J/mol×K	1020.18	Joback Method
cpg	880.38	J/mol×K	1058.05	Joback Method
cpg	888.57	J/mol×K	1095.92	Joback Method
cpg	895.55	J/mol×K	1133.79	Joback Method
cpg	901.37	J/mol×K	1171.66	Joback Method
dvisc	0.0004047	Pa×s	590.63	Joback Method

dvisc	0.0002482	Pa×s	649.60	Joback Method
dvisc	0.0001651	Pa×s	708.57	Joback Method
dvisc	0.0001170	Pa×s	767.53	Joback Method
dvisc	0.0000870	Pa×s	826.50	Joback Method
dvisc	0.0000673	Pa×s	885.47	Joback Method
dvisc	0.0000538	Pa×s	944.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344695&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