Isophthalic acid, 2-formylphenyl octyl ester

Inchi: InChI=1S/C23H26O5/c1-2-3-4-5-6-9-15-27-22(25)18-12-10-13-19(16-18)23(26)28-21-14
InchiKey: QMUNGAAGMVFZGO-UHFFFAOYSA-N
Formula: C23H26O5
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]: 382.45

Physical Properties

Property code	Value	Unit	Source
gf	-219.02	kJ/mol	Joback Method
hf	-643.11	kJ/mol	Joback Method
hfus	50.49	kJ/mol	Joback Method
hvap	97.70	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.236		Crippen Method
mcvol	303.860	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	990.20	K	Joback Method
tc	1218.74	K	Joback Method
tf	613.17	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.35	J/mol×K	990.20	Joback Method
cpg	977.48	J/mol×K	1028.29	Joback Method
cpg	988.22	J/mol×K	1066.38	Joback Method
cpg	997.63	J/mol×K	1104.47	Joback Method
cpg	1005.74	J/mol×K	1142.56	Joback Method
cpg	1012.60	J/mol×K	1180.65	Joback Method
cpg	1018.26	J/mol×K	1218.74	Joback Method
dvisc	0.0003272	Pa×s	613.17	Joback Method

dvisc	0.0001963	Pa×s	676.01	Joback Method
dvisc	0.0001285	Pa×s	738.85	Joback Method
dvisc	0.0000899	Pa×s	801.68	Joback Method
dvisc	0.0000662	Pa×s	864.52	Joback Method
dvisc	0.0000508	Pa×s	927.36	Joback Method
dvisc	0.0000404	Pa×s	990.20	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=U344616&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