Isophthalic acid, 2-formylphenyl propyl ester

Inchi: InChI=1S/C18H16O5/c1-2-10-22-17(20)13-7-5-8-14(11-13)18(21)23-16-9-4-3-6-15(16)12
InchiKey: AFBOUVIRXANXQA-UHFFFAOYSA-N
Formula: C18H16O5
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]: 312.32

Physical Properties

Property code	Value	Unit	Source
gf	-261.12	kJ/mol	Joback Method
hf	-539.91	kJ/mol	Joback Method
hfus	37.54	kJ/mol	Joback Method
hvap	86.57	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.285		Crippen Method
mcvol	233.410	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	875.80	K	Joback Method
tc	1107.05	K	Joback Method
tf	556.82	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.39	J/mol×K	875.80	Joback Method
cpg	689.06	J/mol×K	914.34	Joback Method
cpg	699.51	J/mol×K	952.88	Joback Method
cpg	708.76	J/mol×K	991.43	Joback Method
cpg	716.83	J/mol×K	1029.97	Joback Method
cpg	723.74	J/mol×K	1068.51	Joback Method
cpg	729.54	J/mol×K	1107.05	Joback Method
dvisc	0.0005411	Pa×s	556.82	Joback Method

dvisc	0.0003437	Pa×s	609.98	Joback Method
dvisc	0.0002348	Pa×s	663.15	Joback Method
dvisc	0.0001698	Pa×s	716.31	Joback Method
dvisc	0.0001284	Pa×s	769.47	Joback Method
dvisc	0.0001006	Pa×s	822.64	Joback Method
dvisc	0.0000812	Pa×s	875.80	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=U344611&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