Isophthalic acid, ethyl hex-3-yl ester

Inchi: InChI=1S/C16H22O4/c1-4-8-14(5-2)20-16(18)13-10-7-9-12(11-13)15(17)19-6-3/h7,9-11,
InchiKey: KDBOMMLXIWMVND-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCC(CC)OC(=O)c1cccc(C(=O)OCC)c1
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-283.66	kJ/mol	Joback Method
hf	-643.39	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.599		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	749.28	K	Joback Method
tc	954.00	K	Joback Method
tf	438.34	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.00	J/mol×K	749.28	Joback Method
cpg	715.80	J/mol×K	919.88	Joback Method
cpg	704.40	J/mol×K	885.76	Joback Method
cpg	692.04	J/mol×K	851.64	Joback Method
cpg	678.69	J/mol×K	817.52	Joback Method
cpg	664.35	J/mol×K	783.40	Joback Method
cpg	726.23	J/mol×K	954.00	Joback Method
dvisc	0.0000861	Pa×s	749.28	Joback Method

dvisc	0.0001111	Pa×s	697.46	Joback Method
dvisc	0.0001494	Pa×s	645.63	Joback Method
dvisc	0.0002115	Pa×s	593.81	Joback Method
dvisc	0.0003201	Pa×s	541.99	Joback Method
dvisc	0.0005289	Pa×s	490.16	Joback Method
dvisc	0.0009839	Pa×s	438.34	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=U356494&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