Isophthalic acid, ethyl 1-isopropyl-2-methylpropyl ester

Inchi: InChI=1S/C17H24O4/c1-6-20-16(18)13-8-7-9-14(10-13)17(19)21-15(11(2)3)12(4)5/h7-12

InchiKey: MPJHXBDJBWTCBO-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CCOC(=O)c1cccc(C(=O)OC(C(C)C)C(C)C)c1

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-674.59	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.701		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1962.00		NIST Webbook
tb	771.28	K	Joback Method
tc	980.14	K	Joback Method
tf	419.61	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.98	J/mol×K	771.28	Joback Method
cpg	722.05	J/mol×K	806.09	Joback Method
cpg	737.00	J/mol×K	840.90	Joback Method
cpg	750.84	J/mol×K	875.71	Joback Method
cpg	763.59	J/mol×K	910.52	Joback Method
cpg	775.27	J/mol×K	945.33	Joback Method
cpg	785.88	J/mol×K	980.14	Joback Method
dvisc	0.0012619	Pa×s	419.61	Joback Method
dvisc	0.0005663	Pa×s	478.22	Joback Method

dvisc	0.0003027	Pa×s	536.83	Joback Method
dvisc	0.0001830	Pa×s	595.45	Joback Method
dvisc	0.0001211	Pa×s	654.06	Joback Method
dvisc	0.0000858	Pa×s	712.67	Joback Method
dvisc	0.0000640	Pa×s	771.28	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=U356370&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