Isophthalic acid, ethyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C15H20O4/c1-5-18-14(16)12-7-6-8-13(9-12)15(17)19-11(4)10(2)3/h6-11H,5H2
InchiKey: FARIRUQNOWBQQI-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCOC(=O)c1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-294.52	kJ/mol	Joback Method
hf	-628.03	kJ/mol	Joback Method
hfus	26.79	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.065		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	725.96	K	Joback Method
tc	936.20	K	Joback Method
tf	412.07	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.71	J/mol×K	725.96	Joback Method
cpg	610.01	J/mol×K	761.00	Joback Method
cpg	624.28	J/mol×K	796.04	Joback Method
cpg	637.56	J/mol×K	831.08	Joback Method
cpg	649.83	J/mol×K	866.12	Joback Method
cpg	661.12	J/mol×K	901.16	Joback Method
cpg	671.43	J/mol×K	936.20	Joback Method
dvisc	0.0012644	Pa×s	412.07	Joback Method

dvisc	0.0006354	Pa×s	464.39	Joback Method
dvisc	0.0003670	Pa×s	516.70	Joback Method
dvisc	0.0002345	Pa×s	569.02	Joback Method
dvisc	0.0001616	Pa×s	621.33	Joback Method
dvisc	0.0001180	Pa×s	673.64	Joback Method
dvisc	0.0000901	Pa×s	725.96	Joback Method

Sources

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=U344717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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