Isophthalic acid, 3,4-dimethylphenyl ethyl ester

Inchi: InChI=1S/C18H18O4/c1-4-21-17(19)14-6-5-7-15(11-14)18(20)22-16-9-8-12(2)13(3)10-16

InchiKey: OORVBOJYEGUACW-UHFFFAOYSA-N

Formula: C18H18O4

SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1

Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-171.23	kJ/mol	Joback Method
hf	-465.80	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.699		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	832.12	K	Joback Method
tc	1062.20	K	Joback Method
tf	527.34	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.72	J/mol×K	832.12	Joback Method
cpg	679.47	J/mol×K	870.47	Joback Method
cpg	691.98	J/mol×K	908.81	Joback Method
cpg	703.26	J/mol×K	947.16	Joback Method
cpg	713.33	J/mol×K	985.51	Joback Method
cpg	722.22	J/mol×K	1023.86	Joback Method
cpg	729.93	J/mol×K	1062.20	Joback Method
dvisc	0.0004755	Pa×s	527.34	Joback Method

dvisc	0.0003055	Pa×s	578.14	Joback Method
dvisc	0.0002108	Pa×s	628.93	Joback Method
dvisc	0.0001538	Pa×s	679.73	Joback Method
dvisc	0.0001172	Pa×s	730.53	Joback Method
dvisc	0.0000925	Pa×s	781.32	Joback Method
dvisc	0.0000752	Pa×s	832.12	Joback Method

Sources

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=U344438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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