Isophthalic acid, 3-methylphenyl propyl ester

Inchi: InChI=1S/C18H18O4/c1-3-10-21-17(19)14-7-5-8-15(12-14)18(20)22-16-9-4-6-13(2)11-16
InchiKey: RVVCXMLSERZZPH-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-161.60	kJ/mol	Joback Method
hf	-454.33	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.781		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	827.14	K	Joback Method
tc	1056.49	K	Joback Method
tf	514.82	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.96	J/mol×K	827.14	Joback Method
cpg	680.81	J/mol×K	865.36	Joback Method
cpg	693.42	J/mol×K	903.59	Joback Method
cpg	704.81	J/mol×K	941.81	Joback Method
cpg	715.01	J/mol×K	980.04	Joback Method
cpg	724.04	J/mol×K	1018.26	Joback Method
cpg	731.93	J/mol×K	1056.49	Joback Method
dvisc	0.0005404	Pa×s	514.82	Joback Method

dvisc	0.0003335	Pa×s	566.87	Joback Method
dvisc	0.0002232	Pa×s	618.93	Joback Method
dvisc	0.0001590	Pa×s	670.98	Joback Method
dvisc	0.0001189	Pa×s	723.03	Joback Method
dvisc	0.0000925	Pa×s	775.09	Joback Method
dvisc	0.0000743	Pa×s	827.14	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=U344515&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