Isophthalic acid, 3,4-dimethylphenyl hexyl ester

Inchi: InChI=1S/C22H26O4/c1-4-5-6-7-13-25-21(23)18-9-8-10-19(15-18)22(24)26-20-12-11-16

InchiKey: UKGYATZSMMVQFU-UHFFFAOYSA-N

Formula: C22H26O4

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

Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-137.55	kJ/mol	Joback Method
hf	-548.36	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.260		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	923.64	K	Joback Method
tc	1146.93	K	Joback Method
tf	572.42	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.70	J/mol×K	923.64	Joback Method
cpg	909.81	J/mol×K	960.86	Joback Method
cpg	922.57	J/mol×K	998.07	Joback Method
cpg	934.00	J/mol×K	1035.29	Joback Method
cpg	944.15	J/mol×K	1072.50	Joback Method
cpg	953.03	J/mol×K	1109.72	Joback Method
cpg	960.67	J/mol×K	1146.93	Joback Method
dvisc	0.0003310	Pa×s	572.42	Joback Method

dvisc	0.0002025	Pa×s	630.96	Joback Method
dvisc	0.0001347	Pa×s	689.49	Joback Method
dvisc	0.0000955	Pa×s	748.03	Joback Method
dvisc	0.0000711	Pa×s	806.57	Joback Method
dvisc	0.0000552	Pa×s	865.10	Joback Method
dvisc	0.0000442	Pa×s	923.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344444&Units=SI
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

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