Isophthalic acid, 3,4-dimethylphenyl pentyl ester

Inchi: InChI=1S/C21H24O4/c1-4-5-6-12-24-20(22)17-8-7-9-18(14-17)21(23)25-19-11-10-15(2)1

InchiKey: CCBPFTCHMFINLW-UHFFFAOYSA-N

Formula: C21H24O4

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

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-145.97	kJ/mol	Joback Method
hf	-527.72	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	87.19	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.870		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	900.76	K	Joback Method
tc	1124.68	K	Joback Method
tf	561.15	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.12	J/mol×K	900.76	Joback Method
cpg	851.18	J/mol×K	938.08	Joback Method
cpg	863.92	J/mol×K	975.40	Joback Method
cpg	875.36	J/mol×K	1012.72	Joback Method
cpg	885.54	J/mol×K	1050.04	Joback Method
cpg	894.47	J/mol×K	1087.36	Joback Method
cpg	902.19	J/mol×K	1124.68	Joback Method
dvisc	0.0003648	Pa×s	561.15	Joback Method

dvisc	0.0002258	Pa×s	617.75	Joback Method
dvisc	0.0001515	Pa×s	674.35	Joback Method
dvisc	0.0001081	Pa×s	730.96	Joback Method
dvisc	0.0000810	Pa×s	787.56	Joback Method
dvisc	0.0000631	Pa×s	844.16	Joback Method
dvisc	0.0000507	Pa×s	900.76	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=U344442&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