Isophthalic acid, isohexyl 2-methylphenyl ester

Inchi: InChI=1S/C21H24O4/c1-15(2)8-7-13-24-20(22)17-10-6-11-18(14-17)21(23)25-19-12-5-4

InchiKey: MLEWLVVMRWKDOA-UHFFFAOYSA-N

Formula: C21H24O4

SMILES: Cc1ccccc1OC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-138.78	kJ/mol	Joback Method
hf	-521.53	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	86.14	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.807		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	895.34	K	Joback Method
tc	1121.05	K	Joback Method
tf	533.63	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.74	J/mol×K	895.34	Joback Method
cpg	897.05	J/mol×K	1083.43	Joback Method
cpg	887.95	J/mol×K	1045.81	Joback Method
cpg	877.61	J/mol×K	1008.19	Joback Method
cpg	865.98	J/mol×K	970.58	Joback Method
cpg	853.04	J/mol×K	932.96	Joback Method
cpg	904.93	J/mol×K	1121.05	Joback Method
dvisc	0.0000455	Pa×s	895.34	Joback Method

dvisc	0.0000580	Pa×s	835.06	Joback Method
dvisc	0.0000769	Pa×s	774.77	Joback Method
dvisc	0.0001070	Pa×s	714.49	Joback Method
dvisc	0.0001581	Pa×s	654.20	Joback Method
dvisc	0.0002528	Pa×s	593.91	Joback Method
dvisc	0.0004495	Pa×s	533.63	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=U344349&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