Isophthalic acid, 3,3-dimethylbut-2-yl isohexyl ester

Inchi: InChI=1S/C20H30O4/c1-14(2)9-8-12-23-18(21)16-10-7-11-17(13-16)19(22)24-15(3)20(4
InchiKey: BDAFMVYHSRDAQF-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-249.58	kJ/mol	Joback Method
hf	-739.98	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	79.29	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.871		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	837.13	K	Joback Method
tc	1046.77	K	Joback Method
tf	470.84	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.79	J/mol×K	837.13	Joback Method
cpg	896.41	J/mol×K	872.07	Joback Method
cpg	911.81	J/mol×K	907.01	Joback Method
cpg	926.03	J/mol×K	941.95	Joback Method
cpg	939.11	J/mol×K	976.89	Joback Method
cpg	951.11	J/mol×K	1011.83	Joback Method
cpg	962.05	J/mol×K	1046.77	Joback Method
dvisc	0.0007329	Pa×s	470.84	Joback Method

dvisc	0.0003336	Pa×s	531.89	Joback Method
dvisc	0.0001786	Pa×s	592.94	Joback Method
dvisc	0.0001074	Pa×s	653.99	Joback Method
dvisc	0.0000705	Pa×s	715.03	Joback Method
dvisc	0.0000494	Pa×s	776.08	Joback Method
dvisc	0.0000365	Pa×s	837.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356550&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

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