Terephthalic acid, isohexyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C20H30O4/c1-6-18(15(4)5)24-20(22)17-11-9-16(10-12-17)19(21)23-13-7-8-14

InchiKey: XRBSXPHKLDSMMT-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCC(OC(=O)c1ccc(C(=O)OCCCC(C)C)cc1)C(C)C

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-254.86	kJ/mol	Joback Method
hf	-736.51	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.871		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
rinpol	2308.00		NIST Webbook
tb	839.92	K	Joback Method
tc	1045.58	K	Joback Method
tf	453.42	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/mol×K	839.92	Joback Method
cpg	895.82	J/mol×K	874.20	Joback Method
cpg	911.14	J/mol×K	908.47	Joback Method
cpg	925.26	J/mol×K	942.75	Joback Method
cpg	938.21	J/mol×K	977.03	Joback Method
cpg	950.00	J/mol×K	1011.30	Joback Method
cpg	960.66	J/mol×K	1045.58	Joback Method
dvisc	0.0009099	Pa×s	453.42	Joback Method
dvisc	0.0003967	Pa×s	517.84	Joback Method

dvisc	0.0002078	Pa×s	582.25	Joback Method
dvisc	0.0001239	Pa×s	646.67	Joback Method
dvisc	0.0000811	Pa×s	711.09	Joback Method
dvisc	0.0000569	Pa×s	775.50	Joback Method
dvisc	0.0000422	Pa×s	839.92	Joback Method

Sources

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=U356196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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