Isophthalic acid, di(2-methylcyclohexyl) ester

Inchi: InChI=1S/C22H30O4/c1-15-8-3-5-12-19(15)25-21(23)17-10-7-11-18(14-17)22(24)26-20-
InchiKey: HCBFNDXUODMGQK-UHFFFAOYSA-N
Formula: C22H30O4
SMILES: CC1CCCCC1OC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-197.22	kJ/mol	Joback Method
hf	-693.99	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	86.06	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.158		Crippen Method
mcvol	290.240	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	916.76	K	Joback Method
tc	1156.16	K	Joback Method
tf	527.24	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.17	J/mol×K	916.76	Joback Method
cpg	1014.17	J/mol×K	956.66	Joback Method
cpg	1030.01	J/mol×K	996.56	Joback Method
cpg	1043.70	J/mol×K	1036.46	Joback Method
cpg	1055.29	J/mol×K	1076.36	Joback Method
cpg	1064.82	J/mol×K	1116.26	Joback Method
cpg	1072.30	J/mol×K	1156.16	Joback Method
dvisc	0.0007606	Pa×s	527.24	Joback Method

dvisc	0.0004202	Pa×s	592.16	Joback Method
dvisc	0.0002610	Pa×s	657.08	Joback Method
dvisc	0.0001766	Pa×s	722.00	Joback Method
dvisc	0.0001275	Pa×s	786.92	Joback Method
dvisc	0.0000967	Pa×s	851.84	Joback Method
dvisc	0.0000763	Pa×s	916.76	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=U345757&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