Isophthalic acid, 3,4-dimethylcyclohexyl octyl ester

Inchi: InChI=1S/C24H36O4/c1-4-5-6-7-8-9-15-27-23(25)20-11-10-12-21(17-20)24(26)28-22-14

InchiKey: AYJMQKCDZVRTKZ-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-204.83	kJ/mol	Joback Method
hf	-789.59	kJ/mol	Joback Method
hfus	51.12	kJ/mol	Joback Method
hvap	90.08	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.185		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	942.97	K	Joback Method
tc	1161.49	K	Joback Method
tf	542.40	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.26	J/mol×K	942.97	Joback Method
cpg	1191.88	J/mol×K	1125.07	Joback Method
cpg	1181.55	J/mol×K	1088.65	Joback Method
cpg	1169.55	J/mol×K	1052.23	Joback Method
cpg	1155.86	J/mol×K	1015.81	Joback Method
cpg	1140.44	J/mol×K	979.39	Joback Method
cpg	1200.57	J/mol×K	1161.49	Joback Method
dvisc	0.0000559	Pa×s	942.97	Joback Method

dvisc	0.0000707	Pa×s	876.21	Joback Method
dvisc	0.0000931	Pa×s	809.45	Joback Method
dvisc	0.0001287	Pa×s	742.68	Joback Method
dvisc	0.0001898	Pa×s	675.92	Joback Method
dvisc	0.0003046	Pa×s	609.16	Joback Method
dvisc	0.0005492	Pa×s	542.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343806&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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