

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.26	J/molxK	942.97	Joback Method
cpg	1140.44	J/molxK	979.39	Joback Method
cpg	1155.86	J/molxK	1015.81	Joback Method
cpg	1169.55	J/molxK	1052.23	Joback Method
cpg	1181.55	J/molxK	1088.65	Joback Method
cpg	1191.88	J/molxK	1125.07	Joback Method
cpg	1200.57	J/molxK	1161.49	Joback Method
dvisc	0.0005492	Paxs	542.40	Joback Method

dvisc	0.0003046	Paxs	609.16	Joback Method
dvisc	0.0001898	Paxs	675.92	Joback Method
dvisc	0.0001287	Paxs	742.68	Joback Method
dvisc	0.0000931	Paxs	809.45	Joback Method
dvisc	0.0000707	Paxs	876.21	Joback Method
dvisc	0.0000559	Paxs	942.97	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=U343806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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