

Isophthalic acid, 3,4-dimethylcyclohexyl hexyl ester

Inchi:	InChI=1S/C22H32O4/c1-4-5-6-7-13-25-21(23)18-9-8-10-19(15-18)22(24)26-20-12-11-16
InchiKey:	KVZVDHRRKMLPJU-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-221.67	kJ/mol	Joback Method
hf	-748.31	kJ/mol	Joback Method
hfus	45.94	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.405		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2782.00		NIST Webbook
tb	897.21	K	Joback Method
tc	1114.38	K	Joback Method
tf	519.86	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.89	J/molxK	897.21	Joback Method
cpg	1018.37	J/molxK	933.40	Joback Method
cpg	1034.18	J/molxK	969.60	Joback Method
cpg	1048.36	J/molxK	1005.79	Joback Method
cpg	1060.92	J/molxK	1041.99	Joback Method
cpg	1071.88	J/molxK	1078.18	Joback Method
cpg	1081.28	J/molxK	1114.38	Joback Method
dvisc	0.0006669	Paxs	519.86	Joback Method
dvisc	0.0003784	Paxs	582.75	Joback Method

dvisc	0.0002398	Paxs	645.64	Joback Method
dvisc	0.0001647	Paxs	708.53	Joback Method
dvisc	0.0001203	Paxs	771.43	Joback Method
dvisc	0.0000922	Paxs	834.32	Joback Method
dvisc	0.0000733	Paxs	897.21	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=U343805&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

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