

Isophthalic acid, 3,4-dimethylphenyl octyl ester

Inchi:	InChI=1S/C24H30O4/c1-4-5-6-7-8-9-15-27-23(25)20-11-10-12-21(17-20)24(26)28-22-14
InchiKey:	YRCCNCHBPUGWPX-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-120.71	kJ/mol	Joback Method
hf	-589.64	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.040		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	3109.00		NIST Webbook
tb	969.40	K	Joback Method
tc	1193.86	K	Joback Method
tf	594.96	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.67	J/molxK	969.40	Joback Method
cpg	1071.65	J/molxK	1156.45	Joback Method
cpg	1062.96	J/molxK	1119.04	Joback Method
cpg	1052.96	J/molxK	1081.63	Joback Method
cpg	1041.60	J/molxK	1044.22	Joback Method
cpg	1028.85	J/molxK	1006.81	Joback Method
cpg	1079.05	J/molxK	1193.86	Joback Method
dvisc	0.0000333	Paxs	969.40	Joback Method
dvisc	0.0000419	Paxs	906.99	Joback Method

dvisc	0.0000544	Paxs	844.59	Joback Method
dvisc	0.0000738	Paxs	782.18	Joback Method
dvisc	0.0001054	Paxs	719.77	Joback Method
dvisc	0.0001612	Paxs	657.37	Joback Method
dvisc	0.0002694	Paxs	594.96	Joback Method

Sources

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=U344446&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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