

Isophthalic acid, 3,4-dimethylphenyl dodecyl ester

Inchi:	InChI=1S/C28H38O4/c1-4-5-6-7-8-9-10-11-12-13-19-31-27(29)24-15-14-16-25(21-24)28
InchiKey:	IJWPDSUYBAEQLY-UHFFFAOYSA-N
Formula:	C28H38O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C)c(C)c2)c1
Mol. weight [g/mol]:	438.60

Physical Properties

Property code	Value	Unit	Source
gf	-87.03	kJ/mol	Joback Method
hf	-672.20	kJ/mol	Joback Method
hfus	60.76	kJ/mol	Joback Method
hvap	102.77	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	7.600		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinsol	3523.00		NIST Webbook
tb	1060.92	K	Joback Method
tc	1298.92	K	Joback Method
tf	640.04	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.28	J/molxK	1060.92	Joback Method
cpg	1272.66	J/molxK	1100.59	Joback Method
cpg	1285.36	J/molxK	1140.25	Joback Method
cpg	1296.42	J/molxK	1179.92	Joback Method
cpg	1305.92	J/molxK	1219.59	Joback Method
cpg	1313.92	J/molxK	1259.26	Joback Method
cpg	1320.48	J/molxK	1298.92	Joback Method
dvisc	0.0001715	Paxs	640.04	Joback Method
dvisc	0.0000984	Paxs	710.19	Joback Method

dvisc	0.0000624	Paxs	780.33	Joback Method
dvisc	0.0000427	Paxs	850.48	Joback Method
dvisc	0.0000309	Paxs	920.63	Joback Method
dvisc	0.0000235	Paxs	990.77	Joback Method
dvisc	0.0000185	Paxs	1060.92	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=U344449&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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