

Isophthalic acid, dodecyl phenylethyl ester

Inchi:	InChI=1S/C28H38O4/c1-2-3-4-5-6-7-8-9-10-14-21-31-27(29)25-18-15-19-26(23-25)28(30)
InchiKey:	ALYNKZJDNNWBSM-UHFFFAOYSA-N
Formula:	C28H38O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	438.60

Physical Properties

Property code	Value	Unit	Source
gf	-67.77	kJ/mol	Joback Method
hf	-649.26	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	101.45	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.164		Crippen Method
mvol	372.740	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	3521.00		NIST Webbook
rinpol	3521.00		NIST Webbook
tb	1050.96	K	Joback Method
tc	1286.69	K	Joback Method
tf	615.00	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1260.53	J/molxK	1050.96	Joback Method
cpg	1275.34	J/molxK	1090.25	Joback Method
cpg	1288.56	J/molxK	1129.54	Joback Method
cpg	1300.28	J/molxK	1168.83	Joback Method
cpg	1310.57	J/molxK	1208.11	Joback Method
cpg	1319.51	J/molxK	1247.40	Joback Method
cpg	1327.18	J/molxK	1286.69	Joback Method
dvisc	0.0002110	Paxs	615.00	Joback Method

dvisc	0.0001118	Paxs	687.66	Joback Method
dvisc	0.0000668	Paxs	760.32	Joback Method
dvisc	0.0000437	Paxs	832.98	Joback Method
dvisc	0.0000306	Paxs	905.64	Joback Method
dvisc	0.0000226	Paxs	978.30	Joback Method
dvisc	0.0000174	Paxs	1050.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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