

Isophthalic acid, di(4-tert-butylcyclohexyl) ester

Inchi:	InChI=1S/C28H42O4/c1-27(2,3)21-10-14-23(15-11-21)31-25(29)19-8-7-9-20(18-19)26(30)
InchiKey:	YZHAGBRAHQIVGP-UHFFFAOYSA-N
Formula:	C28H42O4
SMILES:	CC(C)(C)C1CCC(OC(=O)c2cccc(C(=O)OC3CCC(C(C)(C)C)CC3)c2)CC1
Mol. weight [g/mol]:	442.63

Physical Properties

Property code	Value	Unit	Source
gf	-141.02	kJ/mol	Joback Method
hf	-835.33	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	96.82	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.210		Crippen Method
mvol	374.780	ml/mol	McGowan Method
pc	1029.92	kPa	Joback Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook
tb	1047.58	K	Joback Method
tc	1293.90	K	Joback Method
tf	599.70	K	Joback Method
vc	1.385	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1365.65	J/molxK	1047.58	Joback Method
cpg	1382.16	J/molxK	1088.63	Joback Method
cpg	1396.61	J/molxK	1129.69	Joback Method
cpg	1409.11	J/molxK	1170.74	Joback Method
cpg	1419.79	J/molxK	1211.79	Joback Method
cpg	1428.77	J/molxK	1252.84	Joback Method
cpg	1436.19	J/molxK	1293.90	Joback Method
dvisc	0.0002910	Paxs	599.70	Joback Method

dvisc	0.0001417	Paxs	674.35	Joback Method
dvisc	0.0000796	Paxs	748.99	Joback Method
dvisc	0.0000497	Paxs	823.64	Joback Method
dvisc	0.0000335	Paxs	898.29	Joback Method
dvisc	0.0000240	Paxs	972.93	Joback Method
dvisc	0.0000180	Paxs	1047.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345744&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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