

Isophthalic acid, hexyl 4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C24H36O4/c1-5-6-7-8-16-27-22(25)18-10-9-11-19(17-18)23(26)28-21-14-12-2
InchiKey:	OFGIUXAZAVUZFD-UHFFFAOYSA-N
Formula:	C24H36O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	388.54

Physical Properties

Property code	Value	Unit	Source
gf	-194.28	kJ/mol	Joback Method
hf	-778.00	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.185		Crippen Method
mvol	329.280	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
tb	944.41	K	Joback Method
tc	1167.67	K	Joback Method
tf	549.06	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.09	J/molxK	944.41	Joback Method
cpg	1189.31	J/molxK	1130.46	Joback Method
cpg	1178.30	J/molxK	1093.25	Joback Method
cpg	1165.84	J/molxK	1056.04	Joback Method
cpg	1151.86	J/molxK	1018.83	Joback Method
cpg	1136.30	J/molxK	981.62	Joback Method
cpg	1198.92	J/molxK	1167.67	Joback Method
dvisc	0.0000322	Paxs	944.41	Joback Method

dvisc	0.0000422	Paxs	878.52	Joback Method
dvisc	0.0000578	Paxs	812.63	Joback Method
dvisc	0.0000837	Paxs	746.73	Joback Method
dvisc	0.0001302	Paxs	680.84	Joback Method
dvisc	0.0002225	Paxs	614.95	Joback Method
dvisc	0.0004325	Paxs	549.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345738&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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