

Isophthalic acid, isobutyl 4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C22H32O4/c1-15(2)14-25-20(23)16-7-6-8-17(13-16)21(24)26-19-11-9-18(10-1
InchiKey:	MWRZDQZBCICQPL-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-213.56	kJ/mol	Joback Method
hf	-742.00	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.261		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	898.21	K	Joback Method
tc	1124.61	K	Joback Method
tf	511.52	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.73	J/molxK	898.21	Joback Method
cpg	1069.88	J/molxK	1086.87	Joback Method
cpg	1058.55	J/molxK	1049.14	Joback Method
cpg	1045.72	J/molxK	1011.41	Joback Method
cpg	1031.35	J/molxK	973.68	Joback Method
cpg	1015.37	J/molxK	935.94	Joback Method
cpg	1079.78	J/molxK	1124.61	Joback Method
dvisc	0.0000396	Paxs	898.21	Joback Method

dvisc	0.0000524	Paxs	833.76	Joback Method
dvisc	0.0000727	Paxs	769.31	Joback Method
dvisc	0.0001071	Paxs	704.87	Joback Method
dvisc	0.0001705	Paxs	640.42	Joback Method
dvisc	0.0003011	Paxs	575.97	Joback Method
dvisc	0.0006137	Paxs	511.52	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=U345734&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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