Isophthalic acid, ethyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H28O4/c1-5-23-18(21)14-7-6-8-15(13-14)19(22)24-17-11-9-16(10-12-17)2
InchiKey: VVUIPGBCVVHFEF-UHFFFAOYSA-N
Formula: C20H28O4
SMILES: CCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-227.96	kJ/mol	Joback Method
hf	-695.44	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.625		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2501.00		NIST Webbook
rinpol	2501.00		NIST Webbook
tb	852.89	K	Joback Method
tc	1080.23	K	Joback Method
tf	503.98	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.69	J/mol×K	852.89	Joback Method
cpg	950.93	J/mol×K	1042.34	Joback Method
cpg	939.28	J/mol×K	1004.45	Joback Method
cpg	926.18	J/mol×K	966.56	Joback Method
cpg	911.59	J/mol×K	928.67	Joback Method
cpg	895.44	J/mol×K	890.78	Joback Method
cpg	961.18	J/mol×K	1080.23	Joback Method
dvisc	0.0000579	Pa×s	852.89	Joback Method

dvisc	0.0000750	Pa×s	794.74	Joback Method
dvisc	0.0001014	Pa×s	736.59	Joback Method
dvisc	0.0001442	Pa×s	678.43	Joback Method
dvisc	0.0002192	Pa×s	620.28	Joback Method
dvisc	0.0003633	Pa×s	562.13	Joback Method
dvisc	0.0006766	Pa×s	503.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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