Isophthalic acid, butyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C22H32O4/c1-5-6-14-25-20(23)16-8-7-9-17(15-16)21(24)26-19-12-10-18(11-1

InchiKey: PICCGQREHBKOIT-UHFFFAOYSA-N

Formula: C22H32O4

SMILES: CCCCOC(=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	-211.12	kJ/mol	Joback Method
hf	-736.72	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	84.64	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.405		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	898.65	K	Joback Method
tc	1122.47	K	Joback Method
tf	526.52	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.26	J/mol×K	898.65	Joback Method
cpg	1069.07	J/mol×K	1085.17	Joback Method
cpg	1057.70	J/mol×K	1047.86	Joback Method
cpg	1044.90	J/mol×K	1010.56	Joback Method
cpg	1030.59	J/mol×K	973.26	Joback Method
cpg	1014.73	J/mol×K	935.95	Joback Method
cpg	1079.04	J/mol×K	1122.47	Joback Method
dvisc	0.0000434	Pa×s	898.65	Joback Method

dvisc	0.0000566	Pa×s	836.63	Joback Method
dvisc	0.0000769	Pa×s	774.61	Joback Method
dvisc	0.0001105	Pa×s	712.59	Joback Method
dvisc	0.0001699	Pa×s	650.56	Joback Method
dvisc	0.0002861	Pa×s	588.54	Joback Method
dvisc	0.0005448	Pa×s	526.52	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=U345735&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