Isophthalic acid, pentyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C23H34O4/c1-5-6-7-15-26-21(24)17-9-8-10-18(16-17)22(25)27-20-13-11-19(1

InchiKey: WGLQALFWNHMGMD-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-202.70	kJ/mol	Joback Method
hf	-757.36	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.795		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	921.53	K	Joback Method
tc	1144.68	K	Joback Method
tf	537.79	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.92	J/mol×K	921.53	Joback Method
cpg	1128.94	J/mol×K	1107.49	Joback Method
cpg	1117.75	J/mol×K	1070.30	Joback Method
cpg	1105.11	J/mol×K	1033.10	Joback Method
cpg	1090.96	J/mol×K	995.91	Joback Method
cpg	1075.25	J/mol×K	958.72	Joback Method
cpg	1138.74	J/mol×K	1144.68	Joback Method
dvisc	0.0000374	Pa×s	921.53	Joback Method

dvisc	0.0000489	Pa×s	857.57	Joback Method
dvisc	0.0000668	Pa×s	793.62	Joback Method
dvisc	0.0000963	Pa×s	729.66	Joback Method
dvisc	0.0001489	Pa×s	665.70	Joback Method
dvisc	0.0002527	Pa×s	601.75	Joback Method
dvisc	0.0004862	Pa×s	537.79	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=U345736&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