Isophthalic acid, heptyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C25H38O4/c1-5-6-7-8-9-17-28-23(26)19-11-10-12-20(18-19)24(27)29-22-15-1

InchiKey: OBHHQKJWHXWKBL-UHFFFAOYSA-N

Formula: C25H38O4

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

Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-185.86	kJ/mol	Joback Method
hf	-798.64	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	91.32	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.575		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	3026.00		NIST Webbook
rinpol	3026.00		NIST Webbook
tb	967.29	K	Joback Method
tc	1191.51	K	Joback Method
tf	560.33	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.72	J/mol×K	967.29	Joback Method
cpg	1197.81	J/mol×K	1004.66	Joback Method
cpg	1213.24	J/mol×K	1042.03	Joback Method
cpg	1227.06	J/mol×K	1079.40	Joback Method
cpg	1239.34	J/mol×K	1116.77	Joback Method
cpg	1250.15	J/mol×K	1154.14	Joback Method
cpg	1259.56	J/mol×K	1191.51	Joback Method
dvisc	0.0003835	Pa×s	560.33	Joback Method

dvisc	0.0001953	Pa×s	628.16	Joback Method
dvisc	0.0001135	Pa×s	695.98	Joback Method
dvisc	0.0000726	Pa×s	763.81	Joback Method
dvisc	0.0000500	Pa×s	831.64	Joback Method
dvisc	0.0000364	Pa×s	899.46	Joback Method
dvisc	0.0000277	Pa×s	967.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345739&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
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