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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.73	J/mol×K	898.21	Joback Method
cpg	1015.37	J/mol×K	935.94	Joback Method
cpg	1031.35	J/mol×K	973.68	Joback Method
cpg	1045.72	J/mol×K	1011.41	Joback Method
cpg	1058.55	J/mol×K	1049.14	Joback Method
cpg	1069.88	J/mol×K	1086.87	Joback Method
cpg	1079.78	J/mol×K	1124.61	Joback Method
dvisc	0.0006137	Pa×s	511.52	Joback Method

dvisc	0.0003011	Pa×s	575.97	Joback Method
dvisc	0.0001705	Pa×s	640.42	Joback Method
dvisc	0.0001071	Pa×s	704.87	Joback Method
dvisc	0.0000727	Pa×s	769.31	Joback Method
dvisc	0.0000524	Pa×s	833.76	Joback Method
dvisc	0.0000396	Pa×s	898.21	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345734&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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