Phthalic acid, butyl 2-tert-butyl-6-methylphenyl ester

Inchi: InChI=1S/C23H28O4/c1-6-7-15-26-21(24)17-12-8-9-13-18(17)22(25)27-20-16(2)11-10-1

InchiKey: SNCQKZNMDFXKDO-UHFFFAOYSA-N

Formula: C23H28O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)Oc1c(C)cccc1C(C)(C)C

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-126.29	kJ/mol	Joback Method
hf	-577.75	kJ/mol	Joback Method
hfus	40.40	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.469		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	943.29	K	Joback Method
tc	1172.25	K	Joback Method
tf	586.11	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.32	J/mol×K	943.29	Joback Method
cpg	1014.55	J/mol×K	1134.09	Joback Method
cpg	1005.15	J/mol×K	1095.93	Joback Method
cpg	994.59	J/mol×K	1057.77	Joback Method
cpg	982.80	J/mol×K	1019.61	Joback Method
cpg	969.74	J/mol×K	981.45	Joback Method
cpg	1022.84	J/mol×K	1172.25	Joback Method
dvisc	0.0000294	Pa×s	943.29	Joback Method

dvisc	0.0000374	Pa×s	883.76	Joback Method
dvisc	0.0000492	Pa×s	824.23	Joback Method
dvisc	0.0000676	Pa×s	764.70	Joback Method
dvisc	0.0000981	Pa×s	705.17	Joback Method
dvisc	0.0001523	Pa×s	645.64	Joback Method
dvisc	0.0002586	Pa×s	586.11	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=U357095&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