

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

Inchi:	InChI=1S/C23H28O4/c1-15(2)14-26-21(24)17-11-7-8-12-18(17)22(25)27-20-16(3)10-9-1
InchiKey:	YCUVYUWMLDGLRM-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	<chem>Cc1cccc(C(C)(C)C)c1OC(=O)c1cccc1C(=O)OCC(C)C</chem>
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-128.73	kJ/mol	Joback Method
hf	-583.03	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	89.96	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.325		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2504.00		NIST Webbook
tb	942.85	K	Joback Method
tc	1174.13	K	Joback Method
tf	571.11	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.78	J/molxK	942.85	Joback Method
cpg	970.29	J/molxK	981.40	Joback Method
cpg	983.41	J/molxK	1019.94	Joback Method
cpg	995.20	J/molxK	1058.49	Joback Method
cpg	1005.74	J/molxK	1097.03	Joback Method
cpg	1015.07	J/molxK	1135.58	Joback Method
cpg	1023.27	J/molxK	1174.13	Joback Method
dvisc	0.0002810	Paxs	571.11	Joback Method
dvisc	0.0001568	Paxs	633.07	Joback Method

dvisc	0.0000971	Paxs	695.02	Joback Method
dvisc	0.0000650	Paxs	756.98	Joback Method
dvisc	0.0000463	Paxs	818.94	Joback Method
dvisc	0.0000345	Paxs	880.89	Joback Method
dvisc	0.0000268	Paxs	942.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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