

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.92	J/molxK	921.53	Joback Method
cpg	1075.25	J/molxK	958.72	Joback Method
cpg	1090.96	J/molxK	995.91	Joback Method
cpg	1105.11	J/molxK	1033.10	Joback Method
cpg	1117.75	J/molxK	1070.30	Joback Method
cpg	1128.94	J/molxK	1107.49	Joback Method
cpg	1138.74	J/molxK	1144.68	Joback Method
dvisc	0.0004862	Paxs	537.79	Joback Method

dvisc	0.0002527	Paxs	601.75	Joback Method
dvisc	0.0001489	Paxs	665.70	Joback Method
dvisc	0.0000963	Paxs	729.66	Joback Method
dvisc	0.0000668	Paxs	793.62	Joback Method
dvisc	0.0000489	Paxs	857.57	Joback Method
dvisc	0.0000374	Paxs	921.53	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345736&Units=SI

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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