Phthalic acid, isohexyl 2-propylphenyl ester

Inchi: InChI=1S/C23H28O4/c1-4-10-18-12-5-8-15-21(18)27-23(25)20-14-7-6-13-19(20)22(24)2
InchiKey: HOKJUPZVPUZDAL-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCCc1ccccc1OC(=O)c1ccccc1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-121.94	kJ/mol	Joback Method
hf	-562.81	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	90.59	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.451		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	2576.00		NIST Webbook
tb	941.10	K	Joback Method
tc	1165.57	K	Joback Method
tf	556.17	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.42	J/mol×K	941.10	Joback Method
cpg	970.76	J/mol×K	978.51	Joback Method
cpg	983.70	J/mol×K	1015.92	Joback Method
cpg	995.28	J/mol×K	1053.33	Joback Method
cpg	1005.54	J/mol×K	1090.75	Joback Method
cpg	1014.52	J/mol×K	1128.16	Joback Method
cpg	1022.27	J/mol×K	1165.57	Joback Method
dvisc	0.0003644	Pa×s	556.17	Joback Method
dvisc	0.0002004	Pa×s	620.33	Joback Method

dvisc	0.0001233	Pa×s	684.48	Joback Method
dvisc	0.0000824	Pa×s	748.63	Joback Method
dvisc	0.0000587	Pa×s	812.79	Joback Method
dvisc	0.0000440	Pa×s	876.94	Joback Method
dvisc	0.0000343	Pa×s	941.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357021&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