Isophthalic acid, hexyl 2-propylphenyl ester

Inchi: InChI=1S/C23H28O4/c1-3-5-6-9-16-26-22(24)19-13-10-14-20(17-19)23(25)27-21-15-8-7
InchiKey: PDKBSWSMSMCNIN-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CCC)c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-119.50	kJ/mol	Joback Method
hf	-557.53	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.595		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2761.00		NIST Webbook
tb	941.54	K	Joback Method
tc	1164.15	K	Joback Method
tf	571.17	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.96	J/mol×K	941.54	Joback Method
cpg	970.23	J/mol×K	978.64	Joback Method
cpg	983.14	J/mol×K	1015.74	Joback Method
cpg	994.72	J/mol×K	1052.85	Joback Method
cpg	1005.01	J/mol×K	1089.95	Joback Method
cpg	1014.06	J/mol×K	1127.05	Joback Method
cpg	1021.91	J/mol×K	1164.15	Joback Method
dvisc	0.0003350	Pa×s	571.17	Joback Method
dvisc	0.0001947	Pa×s	632.90	Joback Method

dvisc	0.0001247	Pa×s	694.63	Joback Method
dvisc	0.0000858	Pa×s	756.36	Joback Method
dvisc	0.0000625	Pa×s	818.08	Joback Method
dvisc	0.0000476	Pa×s	879.81	Joback Method
dvisc	0.0000376	Pa×s	941.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356629&Units=SI
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

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