Isophthalic acid, hexyl 1-phenylpropyl ester

Inchi: InChI=1S/C23H28O4/c1-3-5-6-10-16-26-22(24)19-14-11-15-20(17-19)23(25)27-21(4-2)1
InchiKey: XUJCLJUHAGVUJI-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(CC)c2ccccc2)c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-112.31	kJ/mol	Joback Method
hf	-551.34	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	89.93	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.732		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2840.00		NIST Webbook
rinpol	2840.00		NIST Webbook
tb	936.12	K	Joback Method
tc	1159.77	K	Joback Method
tf	543.65	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.46	J/mol×K	936.12	Joback Method
cpg	1016.46	J/mol×K	1122.49	Joback Method
cpg	1007.23	J/mol×K	1085.22	Joback Method
cpg	996.76	J/mol×K	1047.94	Joback Method
cpg	985.01	J/mol×K	1010.67	Joback Method
cpg	971.93	J/mol×K	973.39	Joback Method
cpg	1024.50	J/mol×K	1159.77	Joback Method
dvisc	0.0000335	Pa×s	936.12	Joback Method

dvisc	0.0000436	Pa×s	870.71	Joback Method
dvisc	0.0000591	Pa×s	805.30	Joback Method
dvisc	0.0000846	Pa×s	739.88	Joback Method
dvisc	0.0001298	Pa×s	674.47	Joback Method
dvisc	0.0002184	Pa×s	609.06	Joback Method
dvisc	0.0004164	Pa×s	543.65	Joback Method

Sources

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=U344552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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