Isophthalic acid, 2-methylphenyl pentyl ester

Inchi: InChI=1S/C20H22O4/c1-3-4-7-13-23-19(21)16-10-8-11-17(14-16)20(22)24-18-12-6-5-9-1
InchiKey: NXNLJZXUQCLKNY-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)c1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-144.76	kJ/mol	Joback Method
hf	-495.61	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.561		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	872.90	K	Joback Method
tc	1097.43	K	Joback Method
tf	537.36	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.36	J/mol×K	872.90	Joback Method
cpg	794.45	J/mol×K	910.32	Joback Method
cpg	807.26	J/mol×K	947.74	Joback Method
cpg	818.81	J/mol×K	985.17	Joback Method
cpg	829.14	J/mol×K	1022.59	Joback Method
cpg	838.28	J/mol×K	1060.01	Joback Method
cpg	846.26	J/mol×K	1097.43	Joback Method
dvisc	0.0004522	Pa×s	537.36	Joback Method

dvisc	0.0002722	Pa×s	593.28	Joback Method
dvisc	0.0001788	Pa×s	649.21	Joback Method
dvisc	0.0001255	Pa×s	705.13	Joback Method
dvisc	0.0000928	Pa×s	761.05	Joback Method
dvisc	0.0000716	Pa×s	816.98	Joback Method
dvisc	0.0000570	Pa×s	872.90	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=U344348&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