Isophthalic acid, 4-isopropylphenyl pentyl ester

Inchi: InChI=1S/C22H26O4/c1-4-5-6-14-25-21(23)18-8-7-9-19(15-18)22(24)26-20-12-10-17(11

InchiKey: KDXQVXSQAPZNAQ-UHFFFAOYSA-N

Formula: C22H26O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1

Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-130.36	kJ/mol	Joback Method
hf	-542.17	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.376		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	918.22	K	Joback Method
tc	1142.92	K	Joback Method
tf	544.90	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.27	J/mol×K	918.22	Joback Method
cpg	911.59	J/mol×K	955.67	Joback Method
cpg	924.54	J/mol×K	993.12	Joback Method
cpg	936.15	J/mol×K	1030.57	Joback Method
cpg	946.47	J/mol×K	1068.02	Joback Method
cpg	955.52	J/mol×K	1105.47	Joback Method
cpg	963.35	J/mol×K	1142.92	Joback Method
dvisc	0.0004055	Pa×s	544.90	Joback Method

dvisc	0.0002255	Pa×s	607.12	Joback Method
dvisc	0.0001398	Pa×s	669.34	Joback Method
dvisc	0.0000941	Pa×s	731.56	Joback Method
dvisc	0.0000673	Pa×s	793.78	Joback Method
dvisc	0.0000506	Pa×s	856.00	Joback Method
dvisc	0.0000395	Pa×s	918.22	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=U344455&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