Isophthalic acid, 2-ethylphenyl pentyl ester

Inchi: InChI=1S/C21H24O4/c1-3-5-8-14-24-20(22)17-11-9-12-18(15-17)21(23)25-19-13-7-6-10
InchiKey: NYLILUOUARHGLX-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CC)c1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-136.34	kJ/mol	Joback Method
hf	-516.25	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.815		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	895.78	K	Joback Method
tc	1118.92	K	Joback Method
tf	548.63	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.22	J/mol×K	895.78	Joback Method
cpg	852.39	J/mol×K	932.97	Joback Method
cpg	865.25	J/mol×K	970.16	Joback Method
cpg	876.83	J/mol×K	1007.35	Joback Method
cpg	887.18	J/mol×K	1044.54	Joback Method
cpg	896.32	J/mol×K	1081.73	Joback Method
cpg	904.28	J/mol×K	1118.92	Joback Method
dvisc	0.0004108	Pa×s	548.63	Joback Method

dvisc	0.0002443	Pa×s	606.49	Joback Method
dvisc	0.0001591	Pa×s	664.35	Joback Method
dvisc	0.0001109	Pa×s	722.20	Joback Method
dvisc	0.0000816	Pa×s	780.06	Joback Method
dvisc	0.0000626	Pa×s	837.92	Joback Method
dvisc	0.0000498	Pa×s	895.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356763&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

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