Isophthalic acid, di(1-propylbutyl) ester

Inchi: InChI=1S/C22H34O4/c1-5-10-19(11-6-2)25-21(23)17-14-9-15-18(16-17)22(24)26-20(12-
InchiKey: PSJIKPYCRISABS-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCC(CCC)OC(=O)c1cccc(C(=O)OC(CCC)CCC)c1
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-235.58	kJ/mol	Joback Method
hf	-772.51	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.938		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2352.00		NIST Webbook
rinpol	2352.00		NIST Webbook
tb	886.12	K	Joback Method
tc	1091.62	K	Joback Method
tf	490.96	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.25	J/mol×K	886.12	Joback Method
cpg	1014.95	J/mol×K	920.37	Joback Method
cpg	1030.37	J/mol×K	954.62	Joback Method
cpg	1044.54	J/mol×K	988.87	Joback Method
cpg	1057.48	J/mol×K	1023.12	Joback Method
cpg	1069.24	J/mol×K	1057.37	Joback Method
cpg	1079.83	J/mol×K	1091.62	Joback Method
dvisc	0.0006178	Pa×s	490.96	Joback Method

dvisc	0.0002874	Pa×s	556.82	Joback Method
dvisc	0.0001572	Pa×s	622.68	Joback Method
dvisc	0.0000965	Pa×s	688.54	Joback Method
dvisc	0.0000645	Pa×s	754.40	Joback Method
dvisc	0.0000460	Pa×s	820.26	Joback Method
dvisc	0.0000345	Pa×s	886.12	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=U356397&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