Isophthalic acid, butyl oct-3-en-2-yl ester

Inchi: InChI=1S/C20H28O4/c1-4-6-8-9-11-16(3)24-20(22)18-13-10-12-17(15-18)19(21)23-14-7
InchiKey: AHOOAMIATIZZFO-PKNBQFBNSA-N
Formula: C20H28O4
SMILES: CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-169.76	kJ/mol	Joback Method
hf	-608.73	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.935		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	844.96	K	Joback Method
tc	1051.07	K	Joback Method
tf	478.34	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.79	J/mol×K	844.96	Joback Method
cpg	867.60	J/mol×K	879.31	Joback Method
cpg	882.29	J/mol×K	913.66	Joback Method
cpg	895.92	J/mol×K	948.02	Joback Method
cpg	908.51	J/mol×K	982.37	Joback Method
cpg	920.09	J/mol×K	1016.72	Joback Method
cpg	930.72	J/mol×K	1051.07	Joback Method
dvisc	0.0006226	Pa×s	478.34	Joback Method

dvisc	0.0003113	Pa×s	539.44	Joback Method
dvisc	0.0001793	Pa×s	600.55	Joback Method
dvisc	0.0001143	Pa×s	661.65	Joback Method
dvisc	0.0000786	Pa×s	722.75	Joback Method
dvisc	0.0000574	Pa×s	783.86	Joback Method
dvisc	0.0000438	Pa×s	844.96	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=U343892&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