Isophthalic acid, heptyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C20H30O4/c1-5-6-7-8-9-13-23-19(21)17-11-10-12-18(14-17)20(22)24-16(4)15
InchiKey: BOFLGYMVZPOXOJ-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-252.42	kJ/mol	Joback Method
hf	-731.23	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	80.59	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.015		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	840.36	K	Joback Method
tc	1043.99	K	Joback Method
tf	468.42	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/mol×K	840.36	Joback Method
cpg	895.15	J/mol×K	874.30	Joback Method
cpg	910.36	J/mol×K	908.24	Joback Method
cpg	924.40	J/mol×K	942.18	Joback Method
cpg	937.29	J/mol×K	976.12	Joback Method
cpg	949.07	J/mol×K	1010.06	Joback Method
cpg	959.75	J/mol×K	1043.99	Joback Method
dvisc	0.0007750	Pa×s	468.42	Joback Method

dvisc	0.0003677	Pa×s	530.41	Joback Method
dvisc	0.0002040	Pa×s	592.40	Joback Method
dvisc	0.0001265	Pa×s	654.39	Joback Method
dvisc	0.0000852	Pa×s	716.38	Joback Method
dvisc	0.0000611	Pa×s	778.37	Joback Method
dvisc	0.0000460	Pa×s	840.36	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=U344723&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