Isophthalic acid, heptyl neopentyl ester

Inchi: InChI=1S/C20H30O4/c1-5-6-7-8-9-13-23-18(21)16-11-10-12-17(14-16)19(22)24-15-20(2
InchiKey: YUJPVDWYHDOMMC-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-244.70	kJ/mol	Joback Method
hf	-729.42	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.017		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	838.01	K	Joback Method
tc	1043.17	K	Joback Method
tf	500.84	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/mol×K	838.01	Joback Method
cpg	949.13	J/mol×K	1008.98	Joback Method
cpg	937.18	J/mol×K	974.79	Joback Method
cpg	924.22	J/mol×K	940.59	Joback Method
cpg	910.18	J/mol×K	906.40	Joback Method
cpg	895.04	J/mol×K	872.20	Joback Method
cpg	960.08	J/mol×K	1043.17	Joback Method
dvisc	0.0000434	Pa×s	838.01	Joback Method

dvisc	0.0000569	Pa×s	781.82	Joback Method
dvisc	0.0000777	Pa×s	725.62	Joback Method
dvisc	0.0001119	Pa×s	669.42	Joback Method
dvisc	0.0001723	Pa×s	613.23	Joback Method
dvisc	0.0002895	Pa×s	557.03	Joback Method
dvisc	0.0005463	Pa×s	500.84	Joback Method

Sources

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=U343865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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