Isophthalic acid, heptyl pent-4-enyl ester

Inchi: InChI=1S/C20H28O4/c1-3-5-7-8-10-15-24-20(22)18-13-11-12-17(16-18)19(21)23-14-9-6
InchiKey: HZEGGFKQKXDBGD-UHFFFAOYSA-N
Formula: C20H28O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-159.70	kJ/mol	Joback Method
hf	-595.24	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2451.00		NIST Webbook
tb	837.92	K	Joback Method
tc	1039.38	K	Joback Method
tf	496.66	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.45	J/mol×K	837.92	Joback Method
cpg	866.10	J/mol×K	871.50	Joback Method
cpg	880.65	J/mol×K	905.07	Joback Method
cpg	894.14	J/mol×K	938.65	Joback Method
cpg	906.58	J/mol×K	972.22	Joback Method
cpg	918.01	J/mol×K	1005.80	Joback Method
cpg	928.45	J/mol×K	1039.38	Joback Method
dvisc	0.0006053	Pa×s	496.66	Joback Method
dvisc	0.0003358	Pa×s	553.54	Joback Method

dvisc	0.0002080	Pa×s	610.41	Joback Method
dvisc	0.0001397	Pa×s	667.29	Joback Method
dvisc	0.0000999	Pa×s	724.17	Joback Method
dvisc	0.0000751	Pa×s	781.04	Joback Method
dvisc	0.0000586	Pa×s	837.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356717&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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