Isophthalic acid, nonyl pent-4-enyl ester

Inchi: InChI=1S/C22H32O4/c1-3-5-7-8-9-10-12-17-26-22(24)20-15-13-14-19(18-20)21(23)25-1
InchiKey: DMMDKPJDXGMHHN-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCC)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-142.86	kJ/mol	Joback Method
hf	-636.52	kJ/mol	Joback Method
hfus	50.68	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2647.00		NIST Webbook
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tb	883.68	K	Joback Method
tc	1087.55	K	Joback Method
tf	519.20	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.05	J/mol×K	883.68	Joback Method
cpg	1038.00	J/mol×K	1053.57	Joback Method
cpg	1026.45	J/mol×K	1019.59	Joback Method
cpg	1013.81	J/mol×K	985.61	Joback Method
cpg	1000.05	J/mol×K	951.64	Joback Method
cpg	985.14	J/mol×K	917.66	Joback Method
cpg	1048.51	J/mol×K	1087.55	Joback Method
dvisc	0.0000443	Pa×s	883.68	Joback Method

dvisc	0.0000571	Pa×s	822.93	Joback Method
dvisc	0.0000766	Pa×s	762.19	Joback Method
dvisc	0.0001082	Pa×s	701.44	Joback Method
dvisc	0.0001630	Pa×s	640.69	Joback Method
dvisc	0.0002678	Pa×s	579.95	Joback Method
dvisc	0.0004940	Pa×s	519.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356719&Units=SI

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