Isophthalic acid, isohexyl pent-4-enyl ester

Inchi: InChI=1S/C19H26O4/c1-4-5-6-12-22-18(20)16-10-7-11-17(14-16)19(21)23-13-8-9-15(2)3
InchiKey: MGNWETZBCZHXIQ-UHFFFAOYSA-N
Formula: C19H26O4
SMILES: C=CCCCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-170.56	kJ/mol	Joback Method
hf	-579.88	kJ/mol	Joback Method
hfus	39.39	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.403		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2303.00		NIST Webbook
rinpol	2303.00		NIST Webbook
tb	814.60	K	Joback Method
tc	1018.14	K	Joback Method
tf	470.39	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.85	J/mol×K	814.60	Joback Method
cpg	808.44	J/mol×K	848.52	Joback Method
cpg	822.93	J/mol×K	882.45	Joback Method
cpg	836.36	J/mol×K	916.37	Joback Method
cpg	848.74	J/mol×K	950.29	Joback Method
cpg	860.11	J/mol×K	984.22	Joback Method
cpg	870.48	J/mol×K	1018.14	Joback Method
dvisc	0.0007559	Pa×s	470.39	Joback Method

dvisc	0.0003966	Pa×s	527.76	Joback Method
dvisc	0.0002362	Pa×s	585.13	Joback Method
dvisc	0.0001543	Pa×s	642.50	Joback Method
dvisc	0.0001080	Pa×s	699.86	Joback Method
dvisc	0.0000799	Pa×s	757.23	Joback Method
dvisc	0.0000616	Pa×s	814.60	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=U356715&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