Isophthalic acid, hexyl pent-4-enyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-168.12	kJ/mol	Joback Method
hf	-574.60	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.547		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	815.04	K	Joback Method
tc	1016.36	K	Joback Method
tf	485.39	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.31	J/mol×K	815.04	Joback Method
cpg	859.08	J/mol×K	982.80	Joback Method
cpg	847.75	J/mol×K	949.25	Joback Method
cpg	835.43	J/mol×K	915.70	Joback Method
cpg	822.10	J/mol×K	882.15	Joback Method
cpg	807.73	J/mol×K	848.59	Joback Method
cpg	869.46	J/mol×K	1016.36	Joback Method
dvisc	0.0000671	Pa×s	815.04	Joback Method

dvisc	0.0000857	Pa×s	760.10	Joback Method
dvisc	0.0001136	Pa×s	705.16	Joback Method
dvisc	0.0001580	Pa×s	650.21	Joback Method
dvisc	0.0002336	Pa×s	595.27	Joback Method
dvisc	0.0003739	Pa×s	540.33	Joback Method
dvisc	0.0006656	Pa×s	485.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356716&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