Isophthalic acid, octyl trans-hex-3-enyl ester

Inchi: InChI=1S/C22H32O4/c1-3-5-7-9-10-12-17-26-22(24)20-15-13-14-19(18-20)21(23)25-16-
InchiKey: OFUQKMMBLLJYKL-SOFGYWHQSA-N
Formula: C22H32O4
SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCC)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-150.48	kJ/mol	Joback Method
hf	-644.73	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook
tb	891.16	K	Joback Method
tc	1097.33	K	Joback Method
tf	515.88	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.03	J/mol×K	891.16	Joback Method
cpg	1039.58	J/mol×K	1062.97	Joback Method
cpg	1027.80	J/mol×K	1028.61	Joback Method
cpg	1015.00	J/mol×K	994.25	Joback Method
cpg	1001.14	J/mol×K	959.88	Joback Method
cpg	986.16	J/mol×K	925.52	Joback Method
cpg	1050.37	J/mol×K	1097.33	Joback Method
dvisc	0.0000361	Pa×s	891.16	Joback Method

dvisc	0.0000468	Pa×s	828.61	Joback Method
dvisc	0.0000634	Pa×s	766.07	Joback Method
dvisc	0.0000906	Pa×s	703.52	Joback Method
dvisc	0.0001388	Pa×s	640.97	Joback Method
dvisc	0.0002333	Pa×s	578.43	Joback Method
dvisc	0.0004447	Pa×s	515.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356691&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