Di(Z)-non-3-enyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, di(Z)-non-3-enyl ester
Di(Z)-non-3-enyl-1,2-benzenedicarboxylate
Inchi: InChI=1S/C26H38O4/c1-3-5-7-9-11-13-17-21-29-25(27)23-19-15-16-20-24(23)26(28)30-
InchiKey: QKKJDMQLYBFXCG-XSYHWHKQSA-N
Formula: C26H38O4
SMILES: CCCCCC=CCCOC(=O)c1ccccc1C(=O)OCCC=CCCCCC
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-36.58	kJ/mol	Joback Method
hf	-610.07	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	94.64	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.053		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	2947.00		NIST Webbook
tb	986.84	K	Joback Method
tc	1208.20	K	Joback Method
tf	555.88	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.80	J/mol×K	986.84	Joback Method
cpg	1203.78	J/mol×K	1023.73	Joback Method
cpg	1219.54	J/mol×K	1060.63	Joback Method
cpg	1234.16	J/mol×K	1097.52	Joback Method
cpg	1247.73	J/mol×K	1134.42	Joback Method
cpg	1260.33	J/mol×K	1171.31	Joback Method
cpg	1272.03	J/mol×K	1208.20	Joback Method

dvisc	0.0002600	Pa×s	555.88	Joback Method
dvisc	0.0001284	Pa×s	627.71	Joback Method
dvisc	0.0000732	Pa×s	699.53	Joback Method
dvisc	0.0000464	Pa×s	771.36	Joback Method
dvisc	0.0000318	Pa×s	843.19	Joback Method
dvisc	0.0000231	Pa×s	915.01	Joback Method
dvisc	0.0000176	Pa×s	986.84	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=U373652&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