Di(Z)-hex-3-enyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, di(Z)-hex-3-enyl ester
Di(Z)-hex-3-enyl-1,2-benzenedicarboxylate
Inchi: InChI=1S/C20H26O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6
InchiKey: GQBFYDWVMPDPTM-SFECMWDFSA-N
Formula: C20H26O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)OCCC=CCC
Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-87.10	kJ/mol	Joback Method
hf	-486.23	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	81.28	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.713		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	849.56	K	Joback Method
tc	1058.23	K	Joback Method
tf	488.26	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.64	J/mol×K	849.56	Joback Method
cpg	839.86	J/mol×K	884.34	Joback Method
cpg	854.07	J/mol×K	919.12	Joback Method
cpg	867.31	J/mol×K	953.90	Joback Method
cpg	879.63	J/mol×K	988.67	Joback Method

cpg	891.09	J/mol×K	1023.45	Joback Method
cpg	901.72	J/mol×K	1058.23	Joback Method
dvisc	0.0005054	Pa×s	488.26	Joback Method
dvisc	0.0002654	Pa×s	548.48	Joback Method
dvisc	0.0001583	Pa×s	608.69	Joback Method
dvisc	0.0001036	Pa×s	668.91	Joback Method
dvisc	0.0000727	Pa×s	729.13	Joback Method
dvisc	0.0000539	Pa×s	789.34	Joback Method
dvisc	0.0000417	Pa×s	849.56	Joback Method

Sources

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=U373650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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