

Di(E)-hex-3-enyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, di(E)-hex-3-enyl ester Di(E)-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-KQQUZDAGSA-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	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2342.00		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/molxK	849.56	Joback Method
cpg	891.09	J/molxK	1023.45	Joback Method
cpg	879.63	J/molxK	988.67	Joback Method
cpg	867.31	J/molxK	953.90	Joback Method
cpg	854.07	J/molxK	919.12	Joback Method

cpg	839.86	J/molxK	884.34	Joback Method
cpg	901.72	J/molxK	1058.23	Joback Method
dvisc	0.0000417	Paxs	849.56	Joback Method
dvisc	0.0000539	Paxs	789.34	Joback Method
dvisc	0.0000727	Paxs	729.13	Joback Method
dvisc	0.0001036	Paxs	668.91	Joback Method
dvisc	0.0001583	Paxs	608.69	Joback Method
dvisc	0.0002654	Paxs	548.48	Joback Method
dvisc	0.0005054	Paxs	488.26	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=U373648&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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