

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

Inchi:	InChI=1S/C20H28O4/c1-4-5-6-7-13-23-19(21)17-11-8-12-18(15-17)20(22)24-14-9-10-16
InchiKey:	WKAUDIAUJJOXYSZ-AATRIKPKSA-N
Formula:	C20H28O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-169.76	kJ/mol	Joback Method
hf	-608.73	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.793		Crippen Method
mvol	279.480	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2394.00		NIST Webbook
tb	844.96	K	Joback Method
tc	1051.07	K	Joback Method
tf	478.34	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.79	J/molxK	844.96	Joback Method
cpg	867.60	J/molxK	879.31	Joback Method
cpg	882.29	J/molxK	913.66	Joback Method
cpg	895.92	J/molxK	948.02	Joback Method
cpg	908.51	J/molxK	982.37	Joback Method
cpg	920.09	J/molxK	1016.72	Joback Method
cpg	930.72	J/molxK	1051.07	Joback Method
dvisc	0.0006226	Paxs	478.34	Joback Method
dvisc	0.0003113	Paxs	539.44	Joback Method

dvisc	0.0001793	Paxs	600.55	Joback Method
dvisc	0.0001143	Paxs	661.65	Joback Method
dvisc	0.0000786	Paxs	722.75	Joback Method
dvisc	0.0000574	Paxs	783.86	Joback Method
dvisc	0.0000438	Paxs	844.96	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=U356689&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

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