

Isophthalic acid, isohexyl phenyl ester

Inchi:	InChI=1S/C20H22O4/c1-15(2)8-7-13-23-19(21)16-9-6-10-17(14-16)20(22)24-18-11-4-3-5
InchiKey:	SEUBXFBHYSORJD-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	-137.57	kJ/mol	Joback Method
hf	-489.42	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.499		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	867.48	K	Joback Method
tc	1094.18	K	Joback Method
tf	509.84	K	Joback Method
vc	0.982	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.03	J/molxK	867.48	Joback Method
cpg	796.39	J/molxK	905.26	Joback Method
cpg	809.41	J/molxK	943.05	Joback Method
cpg	821.16	J/molxK	980.83	Joback Method
cpg	831.65	J/molxK	1018.61	Joback Method
cpg	840.94	J/molxK	1056.40	Joback Method
cpg	849.06	J/molxK	1094.18	Joback Method
dvisc	0.0005734	Paxs	509.84	Joback Method

dvisc	0.0003108	Paxs	569.45	Joback Method
dvisc	0.0001892	Paxs	629.05	Joback Method
dvisc	0.0001255	Paxs	688.66	Joback Method
dvisc	0.0000889	Paxs	748.27	Joback Method
dvisc	0.0000662	Paxs	807.87	Joback Method
dvisc	0.0000514	Paxs	867.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U344359&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

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