

Isophthalic acid, isohexyl phenylethyl ester

Inchi:	InChI=1S/C22H26O4/c1-17(2)8-7-14-25-21(23)19-11-6-12-20(16-19)22(24)26-15-13-18-
InchiKey:	GOHQXFIAOMVKJJ-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-120.73	kJ/mol	Joback Method
hf	-530.70	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.679		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2831.00		NIST Webbook
rinpol	2831.00		NIST Webbook
tb	913.24	K	Joback Method
tc	1137.15	K	Joback Method
tf	532.38	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.33	J/molxK	913.24	Joback Method
cpg	957.39	J/molxK	1099.83	Joback Method
cpg	948.11	J/molxK	1062.51	Joback Method
cpg	937.62	J/molxK	1025.20	Joback Method
cpg	925.85	J/molxK	987.88	Joback Method
cpg	912.77	J/molxK	950.56	Joback Method
cpg	965.49	J/molxK	1137.15	Joback Method
dvisc	0.0000388	Paxs	913.24	Joback Method

dvisc	0.0000502	Paxs	849.76	Joback Method
dvisc	0.0000679	Paxs	786.29	Joback Method
dvisc	0.0000968	Paxs	722.81	Joback Method
dvisc	0.0001477	Paxs	659.33	Joback Method
dvisc	0.0002465	Paxs	595.86	Joback Method
dvisc	0.0004650	Paxs	532.38	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=U344336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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