

Isophthalic acid, heptyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C24H30O5/c1-4-5-6-7-10-16-27-23(25)19-12-11-13-20(17-19)24(26)29-22-15-
InchiKey:	ABJNFWZFDZRXBH-UHFFFAOYSA-N
Formula:	C24H30O5
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]:	398.49

Physical Properties

Property code	Value	Unit	Source
gf	-218.52	kJ/mol	Joback Method
hf	-715.67	kJ/mol	Joback Method
hfus	48.46	kJ/mol	Joback Method
hvap	95.23	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.820		Crippen Method
mvol	322.250	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	986.40	K	Joback Method
tc	1213.19	K	Joback Method
tf	589.67	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.46	J/molxK	986.40	Joback Method
cpg	1094.61	J/molxK	1175.39	Joback Method
cpg	1087.45	J/molxK	1137.60	Joback Method
cpg	1078.79	J/molxK	1099.80	Joback Method
cpg	1068.59	J/molxK	1062.00	Joback Method
cpg	1056.82	J/molxK	1024.20	Joback Method
cpg	1100.29	J/molxK	1213.19	Joback Method
dvisc	0.0000220	Paxs	986.40	Joback Method

dvisc	0.0000282	Paxs	920.28	Joback Method
dvisc	0.0000376	Paxs	854.16	Joback Method
dvisc	0.0000527	Paxs	788.04	Joback Method
dvisc	0.0000786	Paxs	721.91	Joback Method
dvisc	0.0001269	Paxs	655.79	Joback Method
dvisc	0.0002281	Paxs	589.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U344432&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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