

Isophthalic acid, hexyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C21H24O5/c1-3-4-5-6-14-25-20(22)16-8-7-9-17(15-16)21(23)26-19-12-10-18(2)
InchiKey:	QLXJBIKDFSPTCA-UHFFFAOYSA-N
Formula:	C21H24O5
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(OC)cc2)c1
Mol. weight [g/mol]:	356.41

Physical Properties

Property code	Value	Unit	Source
gf	-241.34	kJ/mol	Joback Method
hf	-648.47	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	88.94	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.652		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	918.20	K	Joback Method
tc	1141.23	K	Joback Method
tf	570.86	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.55	J/molxK	918.20	Joback Method
cpg	918.51	J/molxK	1104.05	Joback Method
cpg	910.68	J/molxK	1066.88	Joback Method
cpg	901.49	J/molxK	1029.71	Joback Method
cpg	890.91	J/molxK	992.54	Joback Method
cpg	878.94	J/molxK	955.37	Joback Method
cpg	925.00	J/molxK	1141.23	Joback Method
dvisc	0.0000373	Paxs	918.20	Joback Method

dvisc	0.0000468	Paxs	860.31	Joback Method
dvisc	0.0000608	Paxs	802.42	Joback Method
dvisc	0.0000822	Paxs	744.53	Joback Method
dvisc	0.0001169	Paxs	686.64	Joback Method
dvisc	0.0001774	Paxs	628.75	Joback Method
dvisc	0.0002929	Paxs	570.86	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=U344480&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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