Isophthalic acid, isohexyl 4-methoxyphenyl ester

Inchi: InChI=1S/C21H24O5/c1-15(2)6-5-13-25-20(22)16-7-4-8-17(14-16)21(23)26-19-11-9-18(2

InchiKey: PYVSIZLMLBGAHJ-UHFFFAOYSA-N

Formula: C21H24O5

SMILES: COc1ccc(OC(=O)c2cccc(C(=O)OCCCC(C)C)c2)cc1

Mol. weight [g/mol]: 356.41

Physical Properties

Property code	Value	Unit	Source
gf	-243.78	kJ/mol	Joback Method
hf	-653.75	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	88.55	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.507		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	917.76	K	Joback Method
tc	1143.05	K	Joback Method
tf	555.86	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.06	J/mol×K	917.76	Joback Method
cpg	879.54	J/mol×K	955.31	Joback Method
cpg	891.56	J/mol×K	992.86	Joback Method
cpg	902.14	J/mol×K	1030.40	Joback Method
cpg	911.31	J/mol×K	1067.95	Joback Method
cpg	919.07	J/mol×K	1105.50	Joback Method
cpg	925.45	J/mol×K	1143.05	Joback Method
dvisc	0.0003177	Pa×s	555.86	Joback Method

dvisc	0.0001825	Pa×s	616.18	Joback Method
dvisc	0.0001157	Pa×s	676.49	Joback Method
dvisc	0.0000790	Pa×s	736.81	Joback Method
dvisc	0.0000572	Pa×s	797.13	Joback Method
dvisc	0.0000433	Pa×s	857.44	Joback Method
dvisc	0.0000340	Pa×s	917.76	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=U344479&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