Isophthalic acid, hexyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C21H30O4/c1-3-4-5-8-14-24-20(22)17-11-9-12-18(15-17)21(23)25-19-13-7-6-1

InchiKey: ZASGAFMBSYXEKC-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-222.38	kJ/mol	Joback Method
hf	-707.33	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.159		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	879.00	K	Joback Method
tc	1096.93	K	Joback Method
tf	512.83	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.51	J/mol×K	879.00	Joback Method
cpg	953.76	J/mol×K	915.32	Joback Method
cpg	969.45	J/mol×K	951.64	Joback Method
cpg	983.59	J/mol×K	987.96	Joback Method
cpg	996.23	J/mol×K	1024.28	Joback Method
cpg	1007.37	J/mol×K	1060.60	Joback Method
cpg	1017.06	J/mol×K	1096.93	Joback Method
dvisc	0.0006680	Pa×s	512.83	Joback Method

dvisc	0.0003674	Pa×s	573.86	Joback Method
dvisc	0.0002267	Pa×s	634.89	Joback Method
dvisc	0.0001522	Pa×s	695.91	Joback Method
dvisc	0.0001090	Pa×s	756.94	Joback Method
dvisc	0.0000820	Pa×s	817.97	Joback Method
dvisc	0.0000642	Pa×s	879.00	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=U345751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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