Isophthalic acid, 2,5-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C22H26O4/c1-15(2)7-6-12-25-21(23)18-8-5-9-19(14-18)22(24)26-20-13-16(3)1

InchiKey: HGMIBFGECYUHNB-UHFFFAOYSA-N

Formula: C22H26O4

SMILES: Cc1ccc(C)c(OC(=O)c2cccc(C(=O)OCCCC(C)C)c2)c1

Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-139.99	kJ/mol	Joback Method
hf	-553.64	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.116		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	923.20	K	Joback Method
tc	1148.69	K	Joback Method
tf	557.42	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.19	J/mol×K	923.20	Joback Method
cpg	910.39	J/mol×K	960.78	Joback Method
cpg	923.21	J/mol×K	998.36	Joback Method
cpg	934.66	J/mol×K	1035.95	Joback Method
cpg	944.78	J/mol×K	1073.53	Joback Method
cpg	953.59	J/mol×K	1111.11	Joback Method
cpg	961.14	J/mol×K	1148.69	Joback Method
dvisc	0.0003573	Pa×s	557.42	Joback Method

dvisc	0.0002076	Pa×s	618.38	Joback Method
dvisc	0.0001330	Pa×s	679.35	Joback Method
dvisc	0.0000917	Pa×s	740.31	Joback Method
dvisc	0.0000669	Pa×s	801.27	Joback Method
dvisc	0.0000510	Pa×s	862.24	Joback Method
dvisc	0.0000403	Pa×s	923.20	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U344542&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