Isophthalic acid, 3,5-dimethylcyclohexyl propyl ester

Inchi: InChI=1S/C19H26O4/c1-4-8-22-18(20)15-6-5-7-16(12-15)19(21)23-17-10-13(2)9-14(3)11

InchiKey: DVORXJJIBNDCJQ-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CCCOC(=O)c1cccc(C(=O)OC2CC(C)CC(C)C2)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-246.93	kJ/mol	Joback Method
hf	-686.39	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.235		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	828.57	K	Joback Method
tc	1049.29	K	Joback Method
tf	486.05	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.44	J/mol×K	828.57	Joback Method
cpg	839.31	J/mol×K	865.36	Joback Method
cpg	855.60	J/mol×K	902.14	Joback Method
cpg	870.34	J/mol×K	938.93	Joback Method
cpg	883.55	J/mol×K	975.72	Joback Method
cpg	895.22	J/mol×K	1012.50	Joback Method
cpg	905.38	J/mol×K	1049.29	Joback Method
dvisc	0.0008622	Pa×s	486.05	Joback Method

dvisc	0.0005079	Pa×s	543.14	Joback Method
dvisc	0.0003309	Pa×s	600.22	Joback Method
dvisc	0.0002322	Pa×s	657.31	Joback Method
dvisc	0.0001725	Pa×s	714.40	Joback Method
dvisc	0.0001339	Pa×s	771.48	Joback Method
dvisc	0.0001076	Pa×s	828.57	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=U343819&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