

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)1
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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.44	J/mol×K	828.57	Joback Method
cpg	895.22	J/mol×K	1012.50	Joback Method
cpg	883.55	J/mol×K	975.72	Joback Method
cpg	870.34	J/mol×K	938.93	Joback Method
cpg	855.60	J/mol×K	902.14	Joback Method
cpg	839.31	J/mol×K	865.36	Joback Method
cpg	905.38	J/mol×K	1049.29	Joback Method
dvisc	0.0001076	Paxs	828.57	Joback Method

dvisc	0.0001339	Paxs	771.48	Joback Method
dvisc	0.0001725	Paxs	714.40	Joback Method
dvisc	0.0002322	Paxs	657.31	Joback Method
dvisc	0.0003309	Paxs	600.22	Joback Method
dvisc	0.0005079	Paxs	543.14	Joback Method
dvisc	0.0008622	Paxs	486.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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