1,2-Cyclohexanedicarboxylic acid, isobutyl 3-methylphenyl ester

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

InchiKey: GURBRHLBHWXHDO-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: Cc1cccc(OC(=O)C2CCCCC2C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-241.66	kJ/mol	Joback Method
hf	-671.33	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.906		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2279.00		NIST Webbook
tb	832.80	K	Joback Method
tc	1056.75	K	Joback Method
tf	475.29	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.30	J/mol×K	832.80	Joback Method
cpg	891.10	J/mol×K	1019.43	Joback Method
cpg	879.60	J/mol×K	982.10	Joback Method
cpg	866.59	J/mol×K	944.78	Joback Method
cpg	852.05	J/mol×K	907.45	Joback Method
cpg	835.96	J/mol×K	870.13	Joback Method
cpg	901.12	J/mol×K	1056.75	Joback Method
dvisc	0.0000769	Pa×s	832.80	Joback Method
dvisc	0.0000991	Pa×s	773.21	Joback Method

dvisc	0.0001331	Pa×s	713.63	Joback Method
dvisc	0.0001886	Pa×s	654.04	Joback Method
dvisc	0.0002868	Pa×s	594.46	Joback Method
dvisc	0.0004785	Pa×s	534.88	Joback Method
dvisc	0.0009080	Pa×s	475.29	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=U339829&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

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