1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl isobutyl ester

Inchi: InChI=1S/C20H28O4/c1-13(2)12-23-19(21)17-7-5-6-8-18(17)20(22)24-16-10-14(3)9-15(4

InchiKey: FCSROAPLQNWDIW-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: Cc1cc(C)cc(OC(=O)C2CCCCC2C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-242.87	kJ/mol	Joback Method
hf	-703.44	kJ/mol	Joback Method
hfus	35.78	kJ/mol	Joback Method
hvap	81.76	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.214		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	860.66	K	Joback Method
tc	1083.25	K	Joback Method
tf	499.08	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.66	J/mol×K	860.66	Joback Method
cpg	947.92	J/mol×K	1046.15	Joback Method
cpg	936.80	J/mol×K	1009.05	Joback Method
cpg	924.13	J/mol×K	971.96	Joback Method
cpg	909.89	J/mol×K	934.86	Joback Method
cpg	894.08	J/mol×K	897.76	Joback Method
cpg	957.52	J/mol×K	1083.25	Joback Method
dvisc	0.0000684	Pa×s	860.66	Joback Method

dvisc	0.0000871	Pa×s	800.40	Joback Method
dvisc	0.0001156	Pa×s	740.13	Joback Method
dvisc	0.0001612	Pa×s	679.87	Joback Method
dvisc	0.0002397	Pa×s	619.61	Joback Method
dvisc	0.0003884	Pa×s	559.34	Joback Method
dvisc	0.0007071	Pa×s	499.08	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=U339613&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