

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)1
InchiKey:	GURBRHLBHWXHDO-UHFFFAOYSA-N
Formula:	C19H26O4
SMILES:	<chem>Cc1cccc(OC(=O)C2CCCCC2C(=O)OCC(C)C)c1</chem>
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/molxK	832.80	Joback Method
cpg	891.10	J/molxK	1019.43	Joback Method
cpg	879.60	J/molxK	982.10	Joback Method
cpg	866.59	J/molxK	944.78	Joback Method
cpg	852.05	J/molxK	907.45	Joback Method
cpg	835.96	J/molxK	870.13	Joback Method
cpg	901.12	J/molxK	1056.75	Joback Method
dvisc	0.0000769	Paxs	832.80	Joback Method
dvisc	0.0000991	Paxs	773.21	Joback Method

dvisc	0.0001331	Paxs	713.63	Joback Method
dvisc	0.0001886	Paxs	654.04	Joback Method
dvisc	0.0002868	Paxs	594.46	Joback Method
dvisc	0.0004785	Paxs	534.88	Joback Method
dvisc	0.0009080	Paxs	475.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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