

cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi:	InChI=1S/C19H23ClO4/c1-12(2)11-23-18(21)15-6-4-5-7-16(15)19(22)24-14-8-9-17(20)1
InchiKey:	ROZBGGLNLTSSA-UHFFFAOYSA-N
Formula:	C19H23ClO4
SMILES:	Cc1cc(OC(=O)C2CC=CCC2C(=O)OCC(C)C)ccc1Cl
Mol. weight [g/mol]:	350.84

Physical Properties

Property code	Value	Unit	Source
gf	-233.26	kJ/mol	Joback Method
hf	-640.76	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	84.21	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.335		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
tb	874.37	K	Joback Method
tc	1103.57	K	Joback Method
tf	518.49	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.35	J/molxK	874.37	Joback Method
cpg	830.45	J/molxK	912.57	Joback Method
cpg	844.00	J/molxK	950.77	Joback Method
cpg	856.04	J/molxK	988.97	Joback Method
cpg	866.57	J/molxK	1027.17	Joback Method
cpg	875.61	J/molxK	1065.37	Joback Method
cpg	883.20	J/molxK	1103.57	Joback Method
dvisc	0.0006442	Paxs	518.49	Joback Method
dvisc	0.0003732	Paxs	577.80	Joback Method
dvisc	0.0002394	Paxs	637.12	Joback Method

dvisc	0.0001656	Paxs	696.43	Joback Method
dvisc	0.0001214	Paxs	755.74	Joback Method
dvisc	0.0000931	Paxs	815.06	Joback Method
dvisc	0.0000740	Paxs	874.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382647&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/99-739-3/cis-Cyclohex-4-en-1-2-dicarboxylic-acid-4-chloro-3-methylphenyl-isobutyl-ester>

Generated by Cheméo on 2024-05-11 05:13:13.544975201 +0000 UTC m=+17693642.465552528.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.