

1,2-Cyclohexanedicarboxylic acid, isobutyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C19H26O5/c1-13(2)12-23-18(20)16-6-4-5-7-17(16)19(21)24-15-10-8-14(22-3)
InchiKey:	IHUPGFQLABEMFI-UHFFFAOYSA-N
Formula:	C19H26O5
SMILES:	COc1ccc(OC(=O)C2CCCCC2C(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	334.41

Physical Properties

Property code	Value	Unit	Source
gf	-346.66	kJ/mol	Joback Method
hf	-803.55	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	81.28	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.606		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
tb	855.22	K	Joback Method
tc	1077.80	K	Joback Method
tf	497.52	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.45	J/molxK	855.22	Joback Method
cpg	864.26	J/molxK	892.32	Joback Method
cpg	879.44	J/molxK	929.41	Joback Method
cpg	892.98	J/molxK	966.51	Joback Method
cpg	904.89	J/molxK	1003.60	Joback Method
cpg	915.17	J/molxK	1040.70	Joback Method
cpg	923.84	J/molxK	1077.80	Joback Method
dvisc	0.0006408	Paxs	497.52	Joback Method
dvisc	0.0003468	Paxs	557.14	Joback Method
dvisc	0.0002113	Paxs	616.75	Joback Method

dvisc	0.0001405	Paxs	676.37	Joback Method
dvisc	0.0000998	Paxs	735.99	Joback Method
dvisc	0.0000747	Paxs	795.60	Joback Method
dvisc	0.0000581	Paxs	855.22	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=U339668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

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