1,2-Cyclohexanedicarboxylic acid, isobutyl 2-isopropylphenyl ester

Inchi: InChI=1S/C21H30O4/c1-14(2)13-24-20(22)17-10-5-6-11-18(17)21(23)25-19-12-8-7-9-16

InchiKey: ZNBBEVRBWHGRPU-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-227.26	kJ/mol	Joback Method
hf	-717.89	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.721		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	878.12	K	Joback Method
tc	1101.11	K	Joback Method
tf	482.83	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.49	J/mol×K	878.12	Joback Method
cpg	955.09	J/mol×K	915.29	Joback Method
cpg	971.02	J/mol×K	952.45	Joback Method
cpg	985.32	J/mol×K	989.62	Joback Method
cpg	998.00	J/mol×K	1026.78	Joback Method
cpg	1009.11	J/mol×K	1063.95	Joback Method
cpg	1018.67	J/mol×K	1101.11	Joback Method
dvisc	0.0008474	Pa×s	482.83	Joback Method

dvisc	0.0004060	Pa×s	548.71	Joback Method
dvisc	0.0002278	Pa×s	614.59	Joback Method
dvisc	0.0001429	Pa×s	680.47	Joback Method
dvisc	0.0000974	Pa×s	746.36	Joback Method
dvisc	0.0000706	Pa×s	812.24	Joback Method
dvisc	0.0000537	Pa×s	878.12	Joback Method

Sources

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=U339699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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