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

Inchi: InChI=1S/C21H30O4/c1-4-5-14-24-20(22)17-11-6-7-12-18(17)21(23)25-19-13-9-8-10-16

InchiKey: LCENJWAQECFSFJ-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-224.82	kJ/mol	Joback Method
hf	-712.61	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	83.32	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.865		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook
tb	878.56	K	Joback Method
tc	1098.94	K	Joback Method
tf	497.83	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.00	J/mol×K	878.56	Joback Method
cpg	954.42	J/mol×K	915.29	Joback Method
cpg	970.22	J/mol×K	952.02	Joback Method
cpg	984.44	J/mol×K	988.75	Joback Method
cpg	997.10	J/mol×K	1025.48	Joback Method
cpg	1008.23	J/mol×K	1062.21	Joback Method
cpg	1017.85	J/mol×K	1098.94	Joback Method
dvisc	0.0007467	Pa×s	497.83	Joback Method

dvisc	0.0003846	Pa×s	561.28	Joback Method
dvisc	0.0002267	Pa×s	624.74	Joback Method
dvisc	0.0001473	Pa×s	688.19	Joback Method
dvisc	0.0001030	Pa×s	751.65	Joback Method
dvisc	0.0000761	Pa×s	815.11	Joback Method
dvisc	0.0000587	Pa×s	878.56	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=U339700&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