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

Inchi: InChI=1S/C20H28O4/c1-4-13-23-19(21)16-10-5-6-11-17(16)20(22)24-18-12-8-7-9-15(18
InchiKey: KSOXNPOWIOQOJP-UHFFFAOYSA-N
Formula: C20H28O4
SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-233.24	kJ/mol	Joback Method
hf	-691.97	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.475		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	855.68	K	Joback Method
tc	1077.51	K	Joback Method
tf	486.56	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.32	J/mol×K	855.68	Joback Method
cpg	949.40	J/mol×K	1040.54	Joback Method
cpg	938.07	J/mol×K	1003.57	Joback Method
cpg	925.22	J/mol×K	966.60	Joback Method
cpg	910.82	J/mol×K	929.62	Joback Method
cpg	894.86	J/mol×K	892.65	Joback Method
cpg	959.24	J/mol×K	1077.51	Joback Method
dvisc	0.0000673	Pa×s	855.68	Joback Method

dvisc	0.0000870	Pa×s	794.16	Joback Method
dvisc	0.0001172	Pa×s	732.64	Joback Method
dvisc	0.0001670	Pa×s	671.12	Joback Method
dvisc	0.0002555	Pa×s	609.60	Joback Method
dvisc	0.0004299	Pa×s	548.08	Joback Method
dvisc	0.0008252	Pa×s	486.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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