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

Inchi: InChI=1S/C22H32O4/c1-4-5-10-15-25-21(23)18-12-6-7-13-19(18)22(24)26-20-14-9-8-11

InchiKey: ZVDRJDSQNYINOB-UHFFFAOYSA-N

Formula: C22H32O4

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

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-216.40	kJ/mol	Joback Method
hf	-733.25	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.255		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	901.44	K	Joback Method
tc	1121.08	K	Joback Method
tf	509.10	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.28	J/mol×K	901.44	Joback Method
cpg	1067.56	J/mol×K	1084.47	Joback Method
cpg	1056.66	J/mol×K	1047.87	Joback Method
cpg	1044.22	J/mol×K	1011.26	Joback Method
cpg	1030.19	J/mol×K	974.65	Joback Method
cpg	1014.56	J/mol×K	938.05	Joback Method
cpg	1076.93	J/mol×K	1121.08	Joback Method
dvisc	0.0000511	Pa×s	901.44	Joback Method

dvisc	0.0000664	Pa×s	836.05	Joback Method
dvisc	0.0000901	Pa×s	770.66	Joback Method
dvisc	0.0001295	Pa×s	705.27	Joback Method
dvisc	0.0002005	Pa×s	639.88	Joback Method
dvisc	0.0003428	Pa×s	574.49	Joback Method
dvisc	0.0006727	Pa×s	509.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339701&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

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