1,2-Cyclohexanedicarboxylic acid, heptyl 4-isopropylphenyl ester

Inchi: InChI=1S/C24H36O4/c1-4-5-6-7-10-17-27-23(25)21-11-8-9-12-22(21)24(26)28-20-15-13

InchiKey: RQIWLLWENZLDQT-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(C(C)C)cc1

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-199.56	kJ/mol	Joback Method
hf	-774.53	kJ/mol	Joback Method
hfus	46.52	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.035		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	947.20	K	Joback Method
tc	1167.68	K	Joback Method
tf	531.64	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.38	J/mol×K	947.20	Joback Method
cpg	1136.37	J/mol×K	983.95	Joback Method
cpg	1151.65	J/mol×K	1020.69	Joback Method
cpg	1165.24	J/mol×K	1057.44	Joback Method
cpg	1177.19	J/mol×K	1094.19	Joback Method
cpg	1187.53	J/mol×K	1130.93	Joback Method
cpg	1196.30	J/mol×K	1167.68	Joback Method

dvisc	0.0005399	Pa×s	531.64	Joback Method
dvisc	0.0002696	Pa×s	600.90	Joback Method
dvisc	0.0001554	Pa×s	670.16	Joback Method
dvisc	0.0000993	Pa×s	739.42	Joback Method
dvisc	0.0000685	Pa×s	808.68	Joback Method
dvisc	0.0000501	Pa×s	877.94	Joback Method
dvisc	0.0000384	Pa×s	947.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339609&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