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

Inchi: InChI=1S/C23H34O4/c1-4-5-6-11-16-26-22(24)19-13-7-8-14-20(19)23(25)27-21-15-10-9

InchiKey: PEQLTOOOUBCFSJ-UHFFFAOYSA-N

Formula: C23H34O4

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

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-207.98	kJ/mol	Joback Method
hf	-753.89	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	87.77	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.645		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	924.32	K	Joback Method
tc	1143.98	K	Joback Method
tf	520.37	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.09	J/mol×K	924.32	Joback Method
cpg	1075.23	J/mol×K	960.93	Joback Method
cpg	1090.69	J/mol×K	997.54	Joback Method
cpg	1104.50	J/mol×K	1034.15	Joback Method
cpg	1116.70	J/mol×K	1070.76	Joback Method
cpg	1127.34	J/mol×K	1107.37	Joback Method
cpg	1136.43	J/mol×K	1143.98	Joback Method
dvisc	0.0006038	Pa×s	520.37	Joback Method

dvisc	0.0003045	Pa×s	587.69	Joback Method
dvisc	0.0001768	Pa×s	655.02	Joback Method
dvisc	0.0001136	Pa×s	722.35	Joback Method
dvisc	0.0000787	Pa×s	789.67	Joback Method
dvisc	0.0000578	Pa×s	856.99	Joback Method
dvisc	0.0000443	Pa×s	924.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339703&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