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

Inchi: InChI=1S/C23H34O4/c1-16(2)10-9-15-26-22(24)19-12-5-6-13-20(19)23(25)27-21-14-8-7

InchiKey: UIWZXRFCQQXPJD-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-210.42	kJ/mol	Joback Method
hf	-759.17	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.501		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	923.88	K	Joback Method
tc	1145.45	K	Joback Method
tf	505.37	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.54	J/mol×K	923.88	Joback Method
cpg	1075.78	J/mol×K	960.81	Joback Method
cpg	1091.31	J/mol×K	997.74	Joback Method
cpg	1105.15	J/mol×K	1034.67	Joback Method
cpg	1117.34	J/mol×K	1071.59	Joback Method
cpg	1127.91	J/mol×K	1108.52	Joback Method
cpg	1136.91	J/mol×K	1145.45	Joback Method
dvisc	0.0006795	Pa×s	505.37	Joback Method

dvisc	0.0003193	Pa×s	575.12	Joback Method
dvisc	0.0001767	Pa×s	644.87	Joback Method
dvisc	0.0001097	Pa×s	714.62	Joback Method
dvisc	0.0000742	Pa×s	784.38	Joback Method
dvisc	0.0000534	Pa×s	854.13	Joback Method
dvisc	0.0000405	Pa×s	923.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339702&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