1,2-Cyclohexanedicarboxylic acid, di(2-methylcyclohexyl) ester

Inchi: InChI=1S/C22H36O4/c1-15-9-3-7-13-19(15)25-21(23)17-11-5-6-12-18(17)22(24)26-20-1

InchiKey: GWFUSSMLDJQXKE-UHFFFAOYSA-N

Formula: C22H36O4

SMILES: CC1CCCCC1OC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-283.26	kJ/mol	Joback Method
hf	-885.07	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.037		Crippen Method
mcvol	303.140	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	899.98	K	Joback Method
tc	1133.68	K	Joback Method
tf	491.44	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.72	J/mol×K	899.98	Joback Method
cpg	1177.22	J/mol×K	1094.73	Joback Method
cpg	1165.49	J/mol×K	1055.78	Joback Method
cpg	1151.40	J/mol×K	1016.83	Joback Method
cpg	1134.92	J/mol×K	977.88	Joback Method
cpg	1116.04	J/mol×K	938.93	Joback Method
cpg	1186.62	J/mol×K	1133.68	Joback Method
dvisc	0.0000981	Pa×s	899.98	Joback Method

dvisc	0.0001259	Pa×s	831.89	Joback Method
dvisc	0.0001691	Pa×s	763.80	Joback Method
dvisc	0.0002404	Pa×s	695.71	Joback Method
dvisc	0.0003691	Pa×s	627.62	Joback Method
dvisc	0.0006288	Pa×s	559.53	Joback Method
dvisc	0.0012419	Pa×s	491.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339886&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

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