1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl isohexyl ester

Inchi: InChI=1S/C21H36O4/c1-16(2)9-8-14-24-20(22)18-12-6-7-13-19(18)21(23)25-15-17-10-4

InchiKey: AHBIZAPFGDVYCG-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-303.15	kJ/mol	Joback Method
hf	-883.35	kJ/mol	Joback Method
hfus	36.94	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.896		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2452.00		NIST Webbook
rinpol	2452.00		NIST Webbook
tb	866.45	K	Joback Method
tc	1081.84	K	Joback Method
tf	466.27	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.73	J/mol×K	866.45	Joback Method
cpg	1048.99	J/mol×K	902.35	Joback Method
cpg	1067.46	J/mol×K	938.25	Joback Method
cpg	1084.17	J/mol×K	974.14	Joback Method
cpg	1099.14	J/mol×K	1010.04	Joback Method
cpg	1112.41	J/mol×K	1045.94	Joback Method
cpg	1124.01	J/mol×K	1081.84	Joback Method
dvisc	0.0012118	Pa×s	466.27	Joback Method

dvisc	0.0005326	Pa×s	532.97	Joback Method
dvisc	0.0002810	Pa×s	599.66	Joback Method
dvisc	0.0001686	Pa×s	666.36	Joback Method
dvisc	0.0001109	Pa×s	733.06	Joback Method
dvisc	0.0000783	Pa×s	799.75	Joback Method
dvisc	0.0000583	Pa×s	866.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339741&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

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