1,2-Cyclohexanedicarboxylic acid, isohexyl 4-methoxyphenyl ester

Inchi: InChI=1S/C21H30O5/c1-15(2)7-6-14-25-20(22)18-8-4-5-9-19(18)21(23)26-17-12-10-16(2

InchiKey: XGFOFQIRAQSMNY-UHFFFAOYSA-N

Formula: C21H30O5

SMILES: COc1ccc(OC(=O)C2CCCCC2C(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-329.82	kJ/mol	Joback Method
hf	-844.83	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	85.73	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.386		Crippen Method
mcvol	292.880	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	900.98	K	Joback Method
tc	1121.17	K	Joback Method
tf	520.06	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.41	J/mol×K	900.98	Joback Method
cpg	982.90	J/mol×K	937.68	Joback Method
cpg	997.67	J/mol×K	974.38	Joback Method
cpg	1010.75	J/mol×K	1011.08	Joback Method
cpg	1022.14	J/mol×K	1047.78	Joback Method
cpg	1031.85	J/mol×K	1084.47	Joback Method
cpg	1039.90	J/mol×K	1121.17	Joback Method
dvisc	0.0005225	Pa×s	520.06	Joback Method

dvisc	0.0002765	Pa×s	583.55	Joback Method
dvisc	0.0001657	Pa×s	647.03	Joback Method
dvisc	0.0001089	Pa×s	710.52	Joback Method
dvisc	0.0000766	Pa×s	774.01	Joback Method
dvisc	0.0000569	Pa×s	837.49	Joback Method
dvisc	0.0000440	Pa×s	900.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339670&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