

1,2-Cyclohexanedicarboxylic acid, 2,5-dimethylphenyl isohexyl ester

Inchi:	InChI=1S/C22H32O4/c1-15(2)8-7-13-25-21(23)18-9-5-6-10-19(18)22(24)26-20-14-16(3)
InchiKey:	OYCANJDQPOAVHK-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	Cc1ccc(C)c(OC(=O)C2CCCCC2C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-226.03	kJ/mol	Joback Method
hf	-744.72	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.995		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	906.42	K	Joback Method
tc	1126.86	K	Joback Method
tf	521.62	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.65	J/molxK	906.42	Joback Method
cpg	1013.78	J/molxK	943.16	Joback Method
cpg	1029.26	J/molxK	979.90	Joback Method
cpg	1043.10	J/molxK	1016.64	Joback Method
cpg	1055.33	J/molxK	1053.38	Joback Method
cpg	1065.97	J/molxK	1090.12	Joback Method
cpg	1075.05	J/molxK	1126.86	Joback Method
dvisc	0.0005811	Paxs	521.62	Joback Method

dvisc	0.0003119	Paxs	585.75	Joback Method
dvisc	0.0001893	Paxs	649.89	Joback Method
dvisc	0.0001257	Paxs	714.02	Joback Method
dvisc	0.0000893	Paxs	778.15	Joback Method
dvisc	0.0000668	Paxs	842.29	Joback Method
dvisc	0.0000521	Paxs	906.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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