1,2-Cyclohexanedicarboxylic acid, di(3-methylphenyl) ester

Inchi: InChI=1S/C22H24O4/c1-15-7-5-9-17(13-15)25-21(23)19-11-3-4-12-20(19)22(24)26-18-1
InchiKey: NDSUOXWAUCFZEK-UHFFFAOYSA-N
Formula: C22H24O4
SMILES: Cc1cccc(OC(=O)C2CCCCC2C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-111.18	kJ/mol	Joback Method
hf	-502.91	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	88.87	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.621		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	933.54	K	Joback Method
tc	1178.71	K	Joback Method
tf	563.04	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.79	J/mol×K	933.54	Joback Method
cpg	909.63	J/mol×K	974.40	Joback Method
cpg	922.60	J/mol×K	1015.26	Joback Method
cpg	933.75	J/mol×K	1056.13	Joback Method
cpg	943.12	J/mol×K	1096.99	Joback Method
cpg	950.75	J/mol×K	1137.85	Joback Method
cpg	956.69	J/mol×K	1178.71	Joback Method
dvisc	0.0004765	Pa×s	563.04	Joback Method

dvisc	0.0002834	Pa×s	624.79	Joback Method
dvisc	0.0001851	Pa×s	686.54	Joback Method
dvisc	0.0001297	Pa×s	748.29	Joback Method
dvisc	0.0000959	Pa×s	810.04	Joback Method
dvisc	0.0000741	Pa×s	871.79	Joback Method
dvisc	0.0000592	Pa×s	933.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339840&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