1,2-Cyclohexanedicarboxylic acid, di(3,5-dimethylphenyl) ester

Inchi: InChI=1S/C24H28O4/c1-15-9-16(2)12-19(11-15)27-23(25)21-7-5-6-8-22(21)24(26)28-20
InchiKey: XXQPIIKDZSPUSZ-UHFFFAOYSA-N
Formula: C24H28O4
SMILES: Cc1cc(C)cc(OC(=O)C2CCCCC2C(=O)Oc2cc(C)cc(C)c2)c1
Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-113.60	kJ/mol	Joback Method
hf	-567.13	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	94.65	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.238		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2996.00		NIST Webbook
rinpol	2996.00		NIST Webbook
tb	989.26	K	Joback Method
tc	1231.81	K	Joback Method
tf	610.62	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.18	J/mol×K	989.26	Joback Method
cpg	1061.53	J/mol×K	1191.39	Joback Method
cpg	1055.23	J/mol×K	1150.96	Joback Method
cpg	1047.08	J/mol×K	1110.54	Joback Method
cpg	1037.04	J/mol×K	1070.11	Joback Method
cpg	1025.09	J/mol×K	1029.69	Joback Method
cpg	1066.00	J/mol×K	1231.81	Joback Method
dvisc	0.0000472	Pa×s	989.26	Joback Method

dvisc	0.0000583	Pa×s	926.15	Joback Method
dvisc	0.0000741	Pa×s	863.05	Joback Method
dvisc	0.0000979	Pa×s	799.94	Joback Method
dvisc	0.0001356	Pa×s	736.83	Joback Method
dvisc	0.0001997	Pa×s	673.73	Joback Method
dvisc	0.0003186	Pa×s	610.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339623&Units=SI

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