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

Inchi: InChI=1S/C19H26O4/c1-4-11-22-18(20)15-7-5-6-8-16(15)19(21)23-17-12-13(2)9-10-14(1

InchiKey: ZRLVLOXNFAFYJC-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
hfus	39.87	kJ/mol	Joback Method
logp	3.968		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
rinpol	2301.00		NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.85380e+01
Coeff. B	1.59696e+00
Coeff. C	-7.43320e-04
Coeff. D	5.78000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.29857e+01

Coeff. B	2.68640e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	443.15
Temperature range (K), max.	714.11

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339938&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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