1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl propyl ester

Inchi: InChI=1S/C19H26O4/c1-4-9-22-18(20)16-7-5-6-8-17(16)19(21)23-15-11-13(2)10-14(3)12

InchiKey: HRMISBJONQOHMY-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-248.85	kJ/mol	Joback Method
hf	-677.52	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.968		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	838.22	K	Joback Method
tc	1059.81	K	Joback Method
tf	502.81	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.10	J/mol×K	838.22	Joback Method
cpg	888.55	J/mol×K	1022.88	Joback Method
cpg	877.25	J/mol×K	985.94	Joback Method
cpg	864.46	J/mol×K	949.01	Joback Method
cpg	850.18	J/mol×K	912.08	Joback Method
cpg	834.40	J/mol×K	875.15	Joback Method
cpg	898.39	J/mol×K	1059.81	Joback Method
dvisc	0.0000851	Pa×s	838.22	Joback Method

dvisc	0.0001066	Pa×s	782.32	Joback Method
dvisc	0.0001382	Pa×s	726.42	Joback Method
dvisc	0.0001872	Pa×s	670.51	Joback Method
dvisc	0.0002680	Pa×s	614.61	Joback Method
dvisc	0.0004121	Pa×s	558.71	Joback Method
dvisc	0.0006974	Pa×s	502.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339612&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

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