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

Inchi: InChI=1S/C18H24O4/c1-4-21-17(19)15-7-5-6-8-16(15)18(20)22-14-10-12(2)9-13(3)11-14

InchiKey: GCTHIAFBMYWCKT-UHFFFAOYSA-N

Formula: C18H24O4

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

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-257.27	kJ/mol	Joback Method
hf	-656.88	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.578		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	815.34	K	Joback Method
tc	1039.34	K	Joback Method
tf	491.54	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.78	J/mol×K	815.34	Joback Method
cpg	776.13	J/mol×K	852.67	Joback Method
cpg	791.99	J/mol×K	890.01	Joback Method
cpg	806.37	J/mol×K	927.34	Joback Method
cpg	819.27	J/mol×K	964.67	Joback Method
cpg	830.71	J/mol×K	1002.01	Joback Method
cpg	840.69	J/mol×K	1039.34	Joback Method
dvisc	0.0007577	Pa×s	491.54	Joback Method

dvisc	0.0004536	Pa×s	545.51	Joback Method
dvisc	0.0002978	Pa×s	599.47	Joback Method
dvisc	0.0002096	Pa×s	653.44	Joback Method
dvisc	0.0001557	Pa×s	707.41	Joback Method
dvisc	0.0001206	Pa×s	761.37	Joback Method
dvisc	0.0000966	Pa×s	815.34	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=U339611&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