1,2-Cyclohexanedicarboxylic acid, 3-methylphenyl propyl ester

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

InchiKey: WAJUTQNVYACEQR-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-247.64	kJ/mol	Joback Method
hf	-645.41	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.660		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	810.36	K	Joback Method
tc	1033.61	K	Joback Method
tf	479.02	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.48	J/mol×K	810.36	Joback Method
cpg	832.13	J/mol×K	996.40	Joback Method
cpg	820.52	J/mol×K	959.19	Joback Method
cpg	807.47	J/mol×K	921.99	Joback Method
cpg	792.95	J/mol×K	884.78	Joback Method
cpg	776.97	J/mol×K	847.57	Joback Method
cpg	842.31	J/mol×K	1033.61	Joback Method
dvisc	0.0000955	Pa×s	810.36	Joback Method

dvisc	0.0001207	Pa×s	755.14	Joback Method
dvisc	0.0001584	Pa×s	699.91	Joback Method
dvisc	0.0002178	Pa×s	644.69	Joback Method
dvisc	0.0003179	Pa×s	589.47	Joback Method
dvisc	0.0005015	Pa×s	534.24	Joback Method
dvisc	0.0008791	Pa×s	479.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339828&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

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