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

Inchi: InChI=1S/C22H32O4/c1-4-5-6-9-12-25-21(23)19-10-7-8-11-20(19)22(24)26-18-14-16(2)1

InchiKey: NMMOYWHHQOWBCG-UHFFFAOYSA-N

Formula: C22H32O4

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

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-223.59	kJ/mol	Joback Method
hf	-739.44	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.139		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook
tb	906.86	K	Joback Method
tc	1125.21	K	Joback Method
tf	536.62	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.18	J/mol×K	906.86	Joback Method
cpg	1013.19	J/mol×K	943.25	Joback Method
cpg	1028.58	J/mol×K	979.64	Joback Method
cpg	1042.38	J/mol×K	1016.03	Joback Method
cpg	1054.61	J/mol×K	1052.43	Joback Method
cpg	1065.29	J/mol×K	1088.82	Joback Method
cpg	1074.46	J/mol×K	1125.21	Joback Method
dvisc	0.0005283	Pa×s	536.62	Joback Method

dvisc	0.0003011	Pa×s	598.33	Joback Method
dvisc	0.0001906	Pa×s	660.03	Joback Method
dvisc	0.0001305	Pa×s	721.74	Joback Method
dvisc	0.0000948	Pa×s	783.45	Joback Method
dvisc	0.0000722	Pa×s	845.15	Joback Method
dvisc	0.0000570	Pa×s	906.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339616&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