1,2-Cyclohexanedicarboxylic acid, di(5-methoxy-3-methylpentyl) ester

Inchi: InChI=1S/C22H40O6/c1-17(9-13-25-3)11-15-27-21(23)19-7-5-6-8-20(19)22(24)28-16-12

InchiKey: IZOWJPQLTPMKMD-UHFFFAOYSA-N

Formula: C22H40O6

SMILES: COCCC(C)CCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-531.62	kJ/mol	Joback Method
hf	-1228.03	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	87.04	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	4.005		Crippen Method
mcvol	336.600	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	914.18	K	Joback Method
tc	1120.85	K	Joback Method
tf	499.62	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.12	J/mol×K	914.18	Joback Method
cpg	1175.31	J/mol×K	948.62	Joback Method
cpg	1191.75	J/mol×K	983.07	Joback Method
cpg	1206.42	J/mol×K	1017.51	Joback Method
cpg	1219.33	J/mol×K	1051.96	Joback Method
cpg	1230.48	J/mol×K	1086.40	Joback Method
cpg	1239.86	J/mol×K	1120.85	Joback Method
dvisc	0.0004993	Pa×s	499.62	Joback Method

dvisc	0.0002230	Pa×s	568.71	Joback Method
dvisc	0.0001186	Pa×s	637.81	Joback Method
dvisc	0.0000714	Pa×s	706.90	Joback Method
dvisc	0.0000470	Pa×s	775.99	Joback Method
dvisc	0.0000331	Pa×s	845.09	Joback Method
dvisc	0.0000246	Pa×s	914.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339928&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