1,2-Cyclohexanedicarboxylic acid, 2-adamantyl nonyl ester

Inchi: InChI=1S/C27H44O4/c1-2-3-4-5-6-7-10-13-30-26(28)23-11-8-9-12-24(23)27(29)31-25-21

InchiKey: JRLKAAGIKJJHFX-UHFFFAOYSA-N

Formula: C27H44O4

SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-119.91	kJ/mol	Joback Method
hf	-884.67	kJ/mol	Joback Method
hfus	58.61	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.454		Crippen Method
mcvol	362.730	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	3189.00		NIST Webbook
rinpol	3189.00		NIST Webbook
tb	999.77	K	Joback Method
tc	1225.55	K	Joback Method
tf	583.33	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1373.24	J/mol×K	999.77	Joback Method
cpg	1393.85	J/mol×K	1037.40	Joback Method
cpg	1412.92	J/mol×K	1075.03	Joback Method
cpg	1430.56	J/mol×K	1112.66	Joback Method
cpg	1446.90	J/mol×K	1150.29	Joback Method
cpg	1462.04	J/mol×K	1187.92	Joback Method
cpg	1476.13	J/mol×K	1225.55	Joback Method
dvisc	0.0039468	Pa×s	583.33	Joback Method

dvisc	0.0029289	Pa×s	652.74	Joback Method
dvisc	0.0023017	Pa×s	722.14	Joback Method
dvisc	0.0018870	Pa×s	791.55	Joback Method
dvisc	0.0015973	Pa×s	860.96	Joback Method
dvisc	0.0013861	Pa×s	930.36	Joback Method
dvisc	0.0012268	Pa×s	999.77	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=U339774&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