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

Inchi: InChI=1S/C24H38O4/c1-15(2)6-5-9-27-23(25)20-7-3-4-8-21(20)24(26)28-22-18-11-16-10

InchiKey: KLMDXGLBCAHOSU-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-147.61	kJ/mol	Joback Method
hf	-828.03	kJ/mol	Joback Method
hfus	47.32	kJ/mol	Joback Method
hvap	86.36	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.140		Crippen Method
mcvol	320.460	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	930.69	K	Joback Method
tc	1152.48	K	Joback Method
tf	534.52	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.68	J/mol×K	930.69	Joback Method
cpg	1270.42	J/mol×K	1115.52	Joback Method
cpg	1255.38	J/mol×K	1078.55	Joback Method
cpg	1239.08	J/mol×K	1041.59	Joback Method
cpg	1221.44	J/mol×K	1004.62	Joback Method
cpg	1202.34	J/mol×K	967.66	Joback Method
cpg	1284.32	J/mol×K	1152.48	Joback Method
dvisc	0.0015276	Pa×s	930.69	Joback Method

dvisc	0.0017124	Pa×s	864.66	Joback Method
dvisc	0.0019561	Pa×s	798.63	Joback Method
dvisc	0.0022888	Pa×s	732.61	Joback Method
dvisc	0.0027627	Pa×s	666.58	Joback Method
dvisc	0.0034755	Pa×s	600.55	Joback Method
dvisc	0.0046275	Pa×s	534.52	Joback Method

Sources

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=U339770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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