1,2-Cyclohexanedicarboxylic acid, di(2-adamantyl) ester

Inchi: InChI=1S/C28H40O4/c29-27(31-25-19-7-15-5-16(9-19)10-20(25)8-15)23-3-1-2-4-24(23)2

InchiKey: HGEYBOSNLZZANT-UHFFFAOYSA-N

Formula: C28H40O4

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

Mol. weight [g/mol]: 440.61

Physical Properties

Property code	Value	Unit	Source
gf	43.24	kJ/mol	Joback Method
hf	-733.75	kJ/mol	Joback Method
hfus	55.65	kJ/mol	Joback Method
hvap	94.94	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.529		Crippen Method
mcvol	344.240	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3525.00		NIST Webbook
rinpol	3525.00		NIST Webbook
tb	1037.80	K	Joback Method
tc	1282.30	K	Joback Method
tf	636.42	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1401.65	J/mol×K	1037.80	Joback Method
cpg	1507.10	J/mol×K	1241.55	Joback Method
cpg	1487.26	J/mol×K	1200.80	Joback Method
cpg	1467.04	J/mol×K	1160.05	Joback Method
cpg	1446.19	J/mol×K	1119.30	Joback Method
cpg	1424.48	J/mol×K	1078.55	Joback Method
cpg	1526.81	J/mol×K	1282.30	Joback Method
dvisc	0.0583555	Pa×s	1037.80	Joback Method

dvisc	0.0579732	Pa×s	970.90	Joback Method
dvisc	0.0575374	Pa×s	904.01	Joback Method
dvisc	0.0570360	Pa×s	837.11	Joback Method
dvisc	0.0564532	Pa×s	770.21	Joback Method
dvisc	0.0557672	Pa×s	703.32	Joback Method
dvisc	0.0549481	Pa×s	636.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339777&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