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

Inchi: InChI=1S/C24H38O4/c1-2-3-4-7-10-27-23(25)20-8-5-6-9-21(20)24(26)28-22-18-12-16-11

InchiKey: JEMKTABHBQKBBH-UHFFFAOYSA-N

Formula: C24H38O4

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

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-145.17	kJ/mol	Joback Method
hf	-822.75	kJ/mol	Joback Method
hfus	50.84	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.284		Crippen Method
mcvol	320.460	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	931.13	K	Joback Method
tc	1151.10	K	Joback Method
tf	549.52	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.28	J/mol×K	931.13	Joback Method
cpg	1269.75	J/mol×K	1114.44	Joback Method
cpg	1254.69	J/mol×K	1077.78	Joback Method
cpg	1238.42	J/mol×K	1041.12	Joback Method
cpg	1220.83	J/mol×K	1004.45	Joback Method
cpg	1201.82	J/mol×K	967.79	Joback Method
cpg	1283.69	J/mol×K	1151.10	Joback Method
dvisc	0.0016759	Pa×s	931.13	Joback Method

dvisc	0.0018645	Pa×s	867.53	Joback Method
dvisc	0.0021095	Pa×s	803.93	Joback Method
dvisc	0.0024379	Pa×s	740.33	Joback Method
dvisc	0.0028950	Pa×s	676.72	Joback Method
dvisc	0.0035628	Pa×s	613.12	Joback Method
dvisc	0.0046003	Pa×s	549.52	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=U339771&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