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

Inchi: InChI=1S/C23H36O4/c1-2-3-6-9-26-22(24)19-7-4-5-8-20(19)23(25)27-21-17-11-15-10-16
InchiKey: USJQAGNLQGISSN-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-153.59	kJ/mol	Joback Method
hf	-802.11	kJ/mol	Joback Method
hfus	48.25	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.894		Crippen Method
mcvol	306.370	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	908.25	K	Joback Method
tc	1128.00	K	Joback Method
tf	538.25	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.24	J/mol×K	908.25	Joback Method
cpg	1206.97	J/mol×K	1091.38	Joback Method
cpg	1191.89	J/mol×K	1054.75	Joback Method
cpg	1175.57	J/mol×K	1018.13	Joback Method
cpg	1157.92	J/mol×K	981.50	Joback Method
cpg	1138.84	J/mol×K	944.88	Joback Method
cpg	1220.92	J/mol×K	1128.00	Joback Method
dvisc	0.0018437	Pa×s	908.25	Joback Method

dvisc	0.0020397	Pa×s	846.58	Joback Method
dvisc	0.0022926	Pa×s	784.92	Joback Method
dvisc	0.0026288	Pa×s	723.25	Joback Method
dvisc	0.0030922	Pa×s	661.58	Joback Method
dvisc	0.0037607	Pa×s	599.92	Joback Method
dvisc	0.0047836	Pa×s	538.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339769&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