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

Inchi: InChI=1S/C26H42O4/c1-2-3-4-5-6-9-12-29-25(27)22-10-7-8-11-23(22)26(28)30-24-20-14

InchiKey: SQJXYLNCTLYURH-UHFFFAOYSA-N

Formula: C26H42O4

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

Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-128.33	kJ/mol	Joback Method
hf	-864.03	kJ/mol	Joback Method
hfus	56.02	kJ/mol	Joback Method
hvap	91.20	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.064		Crippen Method
mcvol	348.640	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	976.89	K	Joback Method
tc	1199.82	K	Joback Method
tf	572.06	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.82	J/mol×K	976.89	Joback Method
cpg	1397.29	J/mol×K	1162.67	Joback Method
cpg	1382.21	J/mol×K	1125.51	Joback Method
cpg	1365.94	J/mol×K	1088.36	Joback Method
cpg	1348.35	J/mol×K	1051.20	Joback Method
cpg	1329.35	J/mol×K	1014.05	Joback Method
cpg	1411.29	J/mol×K	1199.82	Joback Method
dvisc	0.0013667	Pa×s	976.89	Joback Method

dvisc	0.0015365	Pa×s	909.42	Joback Method
dvisc	0.0017602	Pa×s	841.95	Joback Method
dvisc	0.0020648	Pa×s	774.47	Joback Method
dvisc	0.0024969	Pa×s	707.00	Joback Method
dvisc	0.0031430	Pa×s	639.53	Joback Method
dvisc	0.0041770	Pa×s	572.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339773&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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