1,2-Cyclohexanedicarboxylic acid, pentyl undecyl ester

Inchi: InChI=1S/C24H44O4/c1-3-5-7-8-9-10-11-12-16-20-28-24(26)22-18-14-13-17-21(22)23(2

InchiKey: FUMTZSNXZKSTJX-UHFFFAOYSA-N

Formula: C24H44O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC

Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-299.90	kJ/mol	Joback Method
hf	-994.31	kJ/mol	Joback Method
hfus	56.40	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.600		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	915.98	K	Joback Method
tc	1121.76	K	Joback Method
tf	507.70	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.74	J/mol×K	915.98	Joback Method
cpg	1238.49	J/mol×K	950.28	Joback Method
cpg	1256.64	J/mol×K	984.57	Joback Method
cpg	1273.21	J/mol×K	1018.87	Joback Method
cpg	1288.23	J/mol×K	1053.16	Joback Method
cpg	1301.75	J/mol×K	1087.46	Joback Method
cpg	1313.78	J/mol×K	1121.76	Joback Method
dvisc	0.0006525	Pa×s	507.70	Joback Method

dvisc	0.0003110	Pa×s	575.75	Joback Method
dvisc	0.0001733	Pa×s	643.79	Joback Method
dvisc	0.0001080	Pa×s	711.84	Joback Method
dvisc	0.0000731	Pa×s	779.89	Joback Method
dvisc	0.0000527	Pa×s	847.93	Joback Method
dvisc	0.0000399	Pa×s	915.98	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=U339474&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