1,2-Cyclohexanedicarboxylic acid, allyl undecyl ester

Inchi: InChI=1S/C22H38O4/c1-3-5-6-7-8-9-10-11-14-18-26-22(24)20-16-13-12-15-19(20)21(23
InchiKey: VNCZFWBAAZCFMH-UHFFFAOYSA-N
Formula: C22H38O4
SMILES: C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-228.90	kJ/mol	Joback Method
hf	-827.60	kJ/mol	Joback Method
hfus	49.94	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.596		Crippen Method
mcvol	320.560	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	866.90	K	Joback Method
tc	1066.40	K	Joback Method
tf	483.40	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.76	J/mol×K	866.90	Joback Method
cpg	1146.13	J/mol×K	1033.15	Joback Method
cpg	1132.55	J/mol×K	999.90	Joback Method
cpg	1117.65	J/mol×K	966.65	Joback Method
cpg	1101.40	J/mol×K	933.40	Joback Method
cpg	1083.78	J/mol×K	900.15	Joback Method
cpg	1158.41	J/mol×K	1066.40	Joback Method
dvisc	0.0000572	Pa×s	866.90	Joback Method

dvisc	0.0000748	Pa×s	802.98	Joback Method
dvisc	0.0001026	Pa×s	739.07	Joback Method
dvisc	0.0001494	Pa×s	675.15	Joback Method
dvisc	0.0002351	Pa×s	611.23	Joback Method
dvisc	0.0004115	Pa×s	547.32	Joback Method
dvisc	0.0008353	Pa×s	483.40	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=U339489&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