1,2-Cyclohexanedicarboxylic acid, allyl decyl ester

Inchi: InChI=1S/C21H36O4/c1-3-5-6-7-8-9-10-13-17-25-21(23)19-15-12-11-14-18(19)20(22)24
InchiKey: CBTDOECWCJSHTQ-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-237.32	kJ/mol	Joback Method
hf	-806.96	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	80.10	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.206		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	844.02	K	Joback Method
tc	1041.73	K	Joback Method
tf	472.13	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.17	J/mol×K	844.02	Joback Method
cpg	1084.52	J/mol×K	1008.78	Joback Method
cpg	1070.84	J/mol×K	975.82	Joback Method
cpg	1055.89	J/mol×K	942.87	Joback Method
cpg	1039.65	J/mol×K	909.92	Joback Method
cpg	1022.08	J/mol×K	876.97	Joback Method
cpg	1096.95	J/mol×K	1041.73	Joback Method
dvisc	0.0000658	Pa×s	844.02	Joback Method

dvisc	0.0000859	Pa×s	782.04	Joback Method
dvisc	0.0001173	Pa×s	720.06	Joback Method
dvisc	0.0001700	Pa×s	658.08	Joback Method
dvisc	0.0002661	Pa×s	596.09	Joback Method
dvisc	0.0004622	Pa×s	534.11	Joback Method
dvisc	0.0009279	Pa×s	472.13	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=U339488&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