1,2-Cyclohexanedicarboxylic acid, allyl tetradecyl ester

Inchi: InChI=1S/C25H44O4/c1-3-5-6-7-8-9-10-11-12-13-14-17-21-29-25(27)23-19-16-15-18-22

InchiKey: CYKPSSFQSQIYAJ-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCCCCCCCC

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-203.64	kJ/mol	Joback Method
hf	-889.52	kJ/mol	Joback Method
hfus	57.71	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.766		Crippen Method
mcvol	362.830	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
rinpol	2844.00		NIST Webbook
rinpol	2844.00		NIST Webbook
tb	935.54	K	Joback Method
tc	1145.41	K	Joback Method
tf	517.21	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.79	J/mol×K	935.54	Joback Method
cpg	1272.24	J/mol×K	970.52	Joback Method
cpg	1290.06	J/mol×K	1005.50	Joback Method
cpg	1306.29	J/mol×K	1040.47	Joback Method
cpg	1320.96	J/mol×K	1075.45	Joback Method
cpg	1334.13	J/mol×K	1110.43	Joback Method
cpg	1345.83	J/mol×K	1145.41	Joback Method
dvisc	0.0005955	Pa×s	517.21	Joback Method

dvisc	0.0002847	Pa×s	586.93	Joback Method
dvisc	0.0001592	Pa×s	656.65	Joback Method
dvisc	0.0000996	Pa×s	726.38	Joback Method
dvisc	0.0000676	Pa×s	796.10	Joback Method
dvisc	0.0000488	Pa×s	865.82	Joback Method
dvisc	0.0000370	Pa×s	935.54	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=U339491&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

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