cis-Cyclohex-4-en-1,2-dicarboxylic acid, heptyl undecyl ester

Inchi: InChI=1S/C26H46O4/c1-3-5-7-9-10-11-12-14-18-22-30-26(28)24-20-16-15-19-23(24)25(

InchiKey: XGOOPUMMZAAAHC-UHFFFAOYSA-N

Formula: C26H46O4

SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCC

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-253.10	kJ/mol	Joback Method
hf	-977.81	kJ/mol	Joback Method
hfus	62.80	kJ/mol	Joback Method
hvap	92.19	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.156		Crippen Method
mcvol	376.920	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	960.90	K	Joback Method
tc	1176.90	K	Joback Method
tf	531.00	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.13	J/mol×K	960.90	Joback Method
cpg	1395.22	J/mol×K	1140.90	Joback Method
cpg	1382.54	J/mol×K	1104.90	Joback Method
cpg	1368.23	J/mol×K	1068.90	Joback Method
cpg	1352.26	J/mol×K	1032.90	Joback Method
cpg	1334.58	J/mol×K	996.90	Joback Method
cpg	1406.32	J/mol×K	1176.90	Joback Method
dvisc	0.0000324	Pa×s	960.90	Joback Method

dvisc	0.0000426	Pa×s	889.25	Joback Method
dvisc	0.0000588	Pa×s	817.60	Joback Method
dvisc	0.0000865	Pa×s	745.95	Joback Method
dvisc	0.0001379	Pa×s	674.30	Joback Method
dvisc	0.0002457	Pa×s	602.65	Joback Method
dvisc	0.0005116	Pa×s	531.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382755&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