1,2-Cyclohexanedicarboxylic acid, decyl 4-octyl ester

Inchi: InChI=1S/C26H48O4/c1-4-7-9-10-11-12-13-16-21-29-25(27)23-19-14-15-20-24(23)26(28

InchiKey: DHCGSTFAXYGPKW-UHFFFAOYSA-N

Formula: C26H48O4

SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-285.50	kJ/mol	Joback Method
hf	-1040.87	kJ/mol	Joback Method
hfus	58.05	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.379		Crippen Method
mcvol	381.220	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	961.30	K	Joback Method
tc	1177.22	K	Joback Method
tf	515.24	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.53	J/mol×K	961.30	Joback Method
cpg	1366.57	J/mol×K	997.29	Joback Method
cpg	1384.77	J/mol×K	1033.27	Joback Method
cpg	1401.18	J/mol×K	1069.26	Joback Method
cpg	1415.85	J/mol×K	1105.24	Joback Method
cpg	1428.81	J/mol×K	1141.23	Joback Method
cpg	1440.11	J/mol×K	1177.22	Joback Method
dvisc	0.0005807	Pa×s	515.24	Joback Method

dvisc	0.0002521	Pa×s	589.58	Joback Method
dvisc	0.0001319	Pa×s	663.93	Joback Method
dvisc	0.0000787	Pa×s	738.27	Joback Method
dvisc	0.0000516	Pa×s	812.61	Joback Method
dvisc	0.0000363	Pa×s	886.96	Joback Method
dvisc	0.0000269	Pa×s	961.30	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=U339525&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