1,2-Cyclohexanedicarboxylic acid, hexyl undecyl ester

Inchi: InChI=1S/C25H46O4/c1-3-5-7-9-10-11-12-13-17-21-29-25(27)23-19-15-14-18-22(23)24(

InchiKey: VQZLJCHEMIEDSK-UHFFFAOYSA-N

Formula: C25H46O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-291.48	kJ/mol	Joback Method
hf	-1014.95	kJ/mol	Joback Method
hfus	58.99	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.990		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	938.86	K	Joback Method
tc	1149.44	K	Joback Method
tf	518.97	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.28	J/mol×K	938.86	Joback Method
cpg	1302.20	J/mol×K	973.96	Joback Method
cpg	1320.41	J/mol×K	1009.05	Joback Method
cpg	1336.95	J/mol×K	1044.15	Joback Method
cpg	1351.86	J/mol×K	1079.25	Joback Method
cpg	1365.17	J/mol×K	1114.35	Joback Method
cpg	1376.92	J/mol×K	1149.44	Joback Method
dvisc	0.0005793	Pa×s	518.97	Joback Method

dvisc	0.0002735	Pa×s	588.95	Joback Method
dvisc	0.0001515	Pa×s	658.93	Joback Method
dvisc	0.0000939	Pa×s	728.91	Joback Method
dvisc	0.0000634	Pa×s	798.90	Joback Method
dvisc	0.0000455	Pa×s	868.88	Joback Method
dvisc	0.0000344	Pa×s	938.86	Joback Method

Sources

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=U339416&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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