1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl undecyl ester

Inchi: InChI=1S/C25H46O4/c1-5-7-8-9-10-11-12-13-16-19-28-24(26)21-17-14-15-18-22(21)25(

InchiKey: XPAHPUCHQKQVJT-UHFFFAOYSA-N

Formula: C25H46O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-296.36	kJ/mol	Joback Method
hf	-1025.51	kJ/mol	Joback Method
hfus	51.94	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.845		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	937.98	K	Joback Method
tc	1148.53	K	Joback Method
tf	488.97	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.04	J/mol×K	937.98	Joback Method
cpg	1302.89	J/mol×K	973.07	Joback Method
cpg	1321.01	J/mol×K	1008.16	Joback Method
cpg	1337.44	J/mol×K	1043.26	Joback Method
cpg	1352.21	J/mol×K	1078.35	Joback Method
cpg	1365.35	J/mol×K	1113.44	Joback Method
cpg	1376.91	J/mol×K	1148.53	Joback Method
dvisc	0.0007620	Pa×s	488.97	Joback Method

dvisc	0.0003066	Pa×s	563.81	Joback Method
dvisc	0.0001527	Pa×s	638.64	Joback Method
dvisc	0.0000881	Pa×s	713.47	Joback Method
dvisc	0.0000564	Pa×s	788.31	Joback Method
dvisc	0.0000390	Pa×s	863.14	Joback Method
dvisc	0.0000286	Pa×s	937.98	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=U339448&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