1,2-Cyclohexanedicarboxylic acid, 3-methylphenyl undecyl ester

Inchi: InChI=1S/C26H40O4/c1-3-4-5-6-7-8-9-10-13-19-29-25(27)23-17-11-12-18-24(23)26(28)3

InchiKey: DXAVRBYCRMVMPK-UHFFFAOYSA-N

Formula: C26H40O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-180.28	kJ/mol	Joback Method
hf	-810.53	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	94.84	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	6.781		Crippen Method
mcvol	357.460	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	3041.00		NIST Webbook
rinpol	3041.00		NIST Webbook
tb	993.40	K	Joback Method
tc	1217.53	K	Joback Method
tf	569.18	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.81	J/mol×K	993.40	Joback Method
cpg	1308.91	J/mol×K	1180.18	Joback Method
cpg	1299.12	J/mol×K	1142.82	Joback Method
cpg	1287.67	J/mol×K	1105.47	Joback Method
cpg	1274.49	J/mol×K	1068.11	Joback Method
cpg	1259.56	J/mol×K	1030.76	Joback Method
cpg	1317.07	J/mol×K	1217.53	Joback Method
dvisc	0.0000314	Pa×s	993.40	Joback Method

dvisc	0.0000407	Pa×s	922.70	Joback Method
dvisc	0.0000550	Pa×s	851.99	Joback Method
dvisc	0.0000786	Pa×s	781.29	Joback Method
dvisc	0.0001205	Pa×s	710.59	Joback Method
dvisc	0.0002030	Pa×s	639.88	Joback Method
dvisc	0.0003892	Pa×s	569.18	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=U339838&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