1,2-Cyclohexanedicarboxylic acid, cyclobutyl undecyl ester

Inchi: InChI=1S/C23H40O4/c1-2-3-4-5-6-7-8-9-12-18-26-22(24)20-16-10-11-17-21(20)23(25)27

InchiKey: SNAHYTJYRQWBEV-UHFFFAOYSA-N

Formula: C23H40O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCC1

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-259.67	kJ/mol	Joback Method
hf	-907.03	kJ/mol	Joback Method
hfus	49.84	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.963		Crippen Method
mcvol	328.090	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	904.11	K	Joback Method
tc	1112.32	K	Joback Method
tf	510.85	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.81	J/mol×K	904.11	Joback Method
cpg	1226.74	J/mol×K	1077.62	Joback Method
cpg	1213.07	J/mol×K	1042.92	Joback Method
cpg	1197.99	J/mol×K	1008.22	Joback Method
cpg	1181.45	J/mol×K	973.51	Joback Method
cpg	1163.41	J/mol×K	938.81	Joback Method
cpg	1239.04	J/mol×K	1112.32	Joback Method
dvisc	0.0001019	Pa×s	904.11	Joback Method

dvisc	0.0001296	Pa×s	838.57	Joback Method
dvisc	0.0001718	Pa×s	773.02	Joback Method
dvisc	0.0002399	Pa×s	707.48	Joback Method
dvisc	0.0003587	Pa×s	641.94	Joback Method
dvisc	0.0005876	Pa×s	576.39	Joback Method
dvisc	0.0010927	Pa×s	510.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339755&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