1,2-Cyclohexanedicarboxylic acid, cyclobutyl pentadecyl ester

Inchi: InChI=1S/C27H48O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-30-26(28)24-20-14-15-21-25

InchiKey: ZWLIKLJULDPPNT-UHFFFAOYSA-N

Formula: C27H48O4

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

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-225.99	kJ/mol	Joback Method
hf	-989.59	kJ/mol	Joback Method
hfus	60.20	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.523		Crippen Method
mcvol	384.450	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	3107.00		NIST Webbook
rinpol	3107.00		NIST Webbook
tb	995.63	K	Joback Method
tc	1219.16	K	Joback Method
tf	555.93	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.14	J/mol×K	995.63	Joback Method
cpg	1418.03	J/mol×K	1032.88	Joback Method
cpg	1436.07	J/mol×K	1070.14	Joback Method
cpg	1452.35	J/mol×K	1107.39	Joback Method
cpg	1466.93	J/mol×K	1144.65	Joback Method
cpg	1479.89	J/mol×K	1181.90	Joback Method
cpg	1491.30	J/mol×K	1219.16	Joback Method
dvisc	0.0007155	Pa×s	555.93	Joback Method

dvisc	0.0003688	Pa×s	629.21	Joback Method
dvisc	0.0002183	Pa×s	702.50	Joback Method
dvisc	0.0001427	Pa×s	775.78	Joback Method
dvisc	0.0001003	Pa×s	849.06	Joback Method
dvisc	0.0000746	Pa×s	922.35	Joback Method
dvisc	0.0000580	Pa×s	995.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339757&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