1,2-Cyclohexanedicarboxylic acid, cyclobutyl dodecyl ester

Inchi: InChI=1S/C24H42O4/c1-2-3-4-5-6-7-8-9-10-13-19-27-23(25)21-17-11-12-18-22(21)24(26

InchiKey: ONFMCCOXHQUQAO-UHFFFAOYSA-N

Formula: C24H42O4

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

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-251.25	kJ/mol	Joback Method
hf	-927.67	kJ/mol	Joback Method
hfus	52.43	kJ/mol	Joback Method
hvap	87.54	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.353		Crippen Method
mcvol	342.180	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	2776.00		NIST Webbook
rinpol	2776.00		NIST Webbook
tb	926.99	K	Joback Method
tc	1137.63	K	Joback Method
tf	522.12	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.79	J/mol×K	926.99	Joback Method
cpg	1226.42	J/mol×K	962.10	Joback Method
cpg	1244.43	J/mol×K	997.20	Joback Method
cpg	1260.89	J/mol×K	1032.31	Joback Method
cpg	1275.85	J/mol×K	1067.42	Joback Method
cpg	1289.36	J/mol×K	1102.52	Joback Method
cpg	1301.46	J/mol×K	1137.63	Joback Method
dvisc	0.0009885	Pa×s	522.12	Joback Method

dvisc	0.0005257	Pa×s	589.60	Joback Method
dvisc	0.0003183	Pa×s	657.08	Joback Method
dvisc	0.0002116	Pa×s	724.56	Joback Method
dvisc	0.0001508	Pa×s	792.03	Joback Method
dvisc	0.0001133	Pa×s	859.51	Joback Method
dvisc	0.0000888	Pa×s	926.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339756&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

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