

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:	CCCCCCCCCOC(=O)C1CCCC1C(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001296	Paxs	838.57	Joback Method
dvisc	0.0001718	Paxs	773.02	Joback Method
dvisc	0.0002399	Paxs	707.48	Joback Method
dvisc	0.0003587	Paxs	641.94	Joback Method
dvisc	0.0005876	Paxs	576.39	Joback Method
dvisc	0.0010927	Paxs	510.85	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=U339755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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