

1,2-Cyclohexanedicarboxylic acid, methyl tetradecyl ester

Inchi:	InChI=1S/C23H42O4/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-27-23(25)21-18-15-14-17-20(2
InchiKey:	NSBKZTVLCSYVNQ-UHFFFAOYSA-N
Formula:	C23H42O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-308.32	kJ/mol	Joback Method
hf	-973.67	kJ/mol	Joback Method
hfus	53.81	kJ/mol	Joback Method
hvap	85.22	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.210		Crippen Method
mvol	338.950	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	893.10	K	Joback Method
tc	1095.01	K	Joback Method
tf	496.43	K	Joback Method
vc	1.304	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.63	J/molxK	893.10	Joback Method
cpg	1238.73	J/molxK	1061.36	Joback Method
cpg	1225.04	J/molxK	1027.71	Joback Method
cpg	1209.91	J/molxK	994.05	Joback Method
cpg	1193.32	J/molxK	960.40	Joback Method
cpg	1175.24	J/molxK	926.75	Joback Method
cpg	1251.01	J/molxK	1095.01	Joback Method
dvisc	0.0000462	Paxs	893.10	Joback Method

dvisc	0.0000609	Paxs	826.99	Joback Method
dvisc	0.0000842	Paxs	760.88	Joback Method
dvisc	0.0001240	Paxs	694.76	Joback Method
dvisc	0.0001979	Paxs	628.65	Joback Method
dvisc	0.0003525	Paxs	562.54	Joback Method
dvisc	0.0007325	Paxs	496.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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