

1,2-Cyclohexanedicarboxylic acid, methyl nonyl ester

Inchi:	InChI=1S/C18H32O4/c1-3-4-5-6-7-8-11-14-22-18(20)16-13-10-9-12-15(16)17(19)21-2/h
InchiKey:	GMQVRUPLASKXOR-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-350.42	kJ/mol	Joback Method
hf	-870.47	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.260		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	2178.00		NIST Webbook
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tb	778.70	K	Joback Method
tc	973.21	K	Joback Method
tf	440.08	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.78	J/molxK	778.70	Joback Method
cpg	931.83	J/molxK	940.79	Joback Method
cpg	917.63	J/molxK	908.37	Joback Method
cpg	902.23	J/molxK	875.95	Joback Method
cpg	885.63	J/molxK	843.54	Joback Method
cpg	867.82	J/molxK	811.12	Joback Method
cpg	944.86	J/molxK	973.21	Joback Method
dvisc	0.0000926	Paxs	778.70	Joback Method

dvisc	0.0001205	Paxs	722.26	Joback Method
dvisc	0.0001638	Paxs	665.83	Joback Method
dvisc	0.0002358	Paxs	609.39	Joback Method
dvisc	0.0003655	Paxs	552.95	Joback Method
dvisc	0.0006262	Paxs	496.52	Joback Method
dvisc	0.0012314	Paxs	440.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339656&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

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

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