

trans-Cyclohexane-1,3-dicarboxylic acid diethyl ester

Inchi:	InChI=1S/C12H20O4/c1-3-15-11(13)9-6-5-7-10(8-9)12(14)16-4-2/h9-10H,3-8H2,1-2H3/t
InchiKey:	MAQGUOIUBYAVNL-NXEZZACHSA-N
Formula:	C12H20O4
SMILES:	CCOC(=O)C1CCCC(C(=O)OCC)C1
Mol. weight [g/mol]:	228.28
CAS:	62059-57-8

Physical Properties

Property code	Value	Unit	Source
chl	-6639.00 ± 13.00	kJ/mol	NIST Webbook
gf	-400.94	kJ/mol	Joback Method
hf	-746.63	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.919		Crippen Method
mcvol	183.960	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
tb	641.42	K	Joback Method
tc	846.20	K	Joback Method
tf	372.46	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.57	J/molxK	641.42	Joback Method
cpg	527.23	J/molxK	675.55	Joback Method
cpg	543.90	J/molxK	709.68	Joback Method
cpg	559.58	J/molxK	743.81	Joback Method
cpg	574.26	J/molxK	777.94	Joback Method
cpg	587.94	J/molxK	812.07	Joback Method
cpg	600.62	J/molxK	846.20	Joback Method
dvisc	0.0019188	Paxs	372.46	Joback Method

dvisc	0.0010612	Paxs	417.29	Joback Method
dvisc	0.0006584	Paxs	462.11	Joback Method
dvisc	0.0004445	Paxs	506.94	Joback Method
dvisc	0.0003198	Paxs	551.77	Joback Method
dvisc	0.0002418	Paxs	596.59	Joback Method
dvisc	0.0001901	Paxs	641.42	Joback Method

Sources

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=C62059578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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