

1,2-Cyclohexanedicarboxylic acid, trans-

Other names:	trans-1,2-Cyclohexanedicarboxylic Acid trans-Cyclohexane-1,2-dicarboxylic acid
Inchi:	InChI=1S/C8H12O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)/t5-,6-
InchiKey:	QSAWQNUELGIYBC-PHDIDXHHSA-N
Formula:	C8H12O4
SMILES:	O=C(O)C1CCCCC1C(=O)O
Mol. weight [g/mol]:	172.18
CAS:	2305-32-0

Physical Properties

Property code	Value	Unit	Source
chs	-3861.60 ± 0.40	kJ/mol	NIST Webbook
chs	-3892.40 ± 7.50	kJ/mol	NIST Webbook
gf	-498.26	kJ/mol	Joback Method
hf	-704.09	kJ/mol	Joback Method
hfus	20.76	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.962		Crippen Method
mcvol	127.600	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
tb	689.42	K	Joback Method
tc	884.77	K	Joback Method
tf	404.56	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.11	J/molxK	689.42	Joback Method
cpg	375.58	J/molxK	721.98	Joback Method
cpg	385.38	J/molxK	754.54	Joback Method
cpg	394.53	J/molxK	787.09	Joback Method
cpg	403.04	J/molxK	819.65	Joback Method

cpg	410.91	J/mol×K	852.21	Joback Method
cpg	418.18	J/mol×K	884.77	Joback Method
dvisc	0.0040256	Paxs	404.56	Joback Method
dvisc	0.0011364	Paxs	452.04	Joback Method
dvisc	0.0004080	Paxs	499.51	Joback Method
dvisc	0.0001750	Paxs	546.99	Joback Method
dvisc	0.0000859	Paxs	594.47	Joback Method
dvisc	0.0000469	Paxs	641.94	Joback Method
dvisc	0.0000278	Paxs	689.42	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=C2305320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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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