cis-Hexahydroterephthalic acid

Other names: cis-1,4-Cyclohexanedicarboxylic acid
1,4-Cyclohexanedicarboxylic acid, cis-
1,4-Cyclohexanedicarboxylic acid, (Z)-
Inchi: InChI=1S/C8H12O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)/t5-,6+
InchiKey: PXGZQGDTEZPERC-OLQVQODUSA-N
Formula: C8H12O4
SMILES: O=C(O)C1CCC(C(=O)O)CC1
Mol. weight [g/mol]: 172.18
CAS: 619-81-8

Physical Properties

Property code	Value	Unit	Source
chs	-3866.90 ± 0.50	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/mol×K	689.42	Joback Method
cpg	375.58	J/mol×K	721.98	Joback Method
cpg	385.38	J/mol×K	754.54	Joback Method
cpg	394.53	J/mol×K	787.09	Joback Method
cpg	403.04	J/mol×K	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	Pa×s	404.56	Joback Method
dvisc	0.0011364	Pa×s	452.04	Joback Method
dvisc	0.0004080	Pa×s	499.51	Joback Method
dvisc	0.0001750	Pa×s	546.99	Joback Method
dvisc	0.0000859	Pa×s	594.47	Joback Method
dvisc	0.0000469	Pa×s	641.94	Joback Method
dvisc	0.0000278	Pa×s	689.42	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=C619818&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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