

Cyclohexanecarboxylic acid, 4-(1,1-dimethylethyl)-, cis-

Other names: Cyclohexanecarboxylic acid, 4-tert-butyl-, cis-cis-4-tert-Butylcyclohexanecarboxylic acid

Inchi: InChI=1S/C11H20O2/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h8-9H,4-7H2,1-3H3,(H,12,13)/t8

InchiKey: QVQKEGYITJBHRQ-DTORHVGOSA-N

Formula: C11H20O2

SMILES: CC(C)(C)C1CCC(C(=O)O)CC1

Mol. weight [g/mol]: 184.28

CAS: 943-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-204.42	kJ/mol	Joback Method
hf	-509.95	kJ/mol	Joback Method
hfus	15.42	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.924		Crippen Method
mvol	162.430	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	608.78	K	Joback Method
tc	810.89	K	Joback Method
tf	330.04	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.12	J/mol×K	608.78	Joback Method
cpg	521.50	J/mol×K	777.20	Joback Method
cpg	508.50	J/mol×K	743.52	Joback Method
cpg	494.60	J/mol×K	709.83	Joback Method
cpg	479.76	J/mol×K	676.15	Joback Method
cpg	463.95	J/mol×K	642.46	Joback Method
cpg	533.64	J/mol×K	810.89	Joback Method

dvisc	0.0000914	Paxs	608.78	Joback Method
dvisc	0.0001456	Paxs	562.32	Joback Method
dvisc	0.0002522	Paxs	515.87	Joback Method
dvisc	0.0004869	Paxs	469.41	Joback Method
dvisc	0.0010862	Paxs	422.95	Joback Method
dvisc	0.0029539	Paxs	376.50	Joback Method
dvisc	0.0106457	Paxs	330.04	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=C943282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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