

2-Hydroxy-cyclohexanecarboxylic acid ethyl ester, trans

Inchi:	InChI=1S/C9H16O3/c1-2-12-9(11)7-5-3-4-6-8(7)10/h7-8,10H,2-6H2,1H3/t7-,8-/m1/s1
InchiKey:	WOGRTPJVNNCUKN-HTQZYQBOSA-N
Formula:	C9H16O3
SMILES:	CCOC(=O)C1CCCCC1O
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
gf	-329.10	kJ/mol	Joback Method
hf	-592.14	kJ/mol	Joback Method
hfus	18.85	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.101		Crippen Method
mvol	140.120	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	588.67	K	Joback Method
tc	783.67	K	Joback Method
tf	327.31	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.23	J/molxK	588.67	Joback Method
cpg	384.80	J/molxK	621.17	Joback Method
cpg	398.64	J/molxK	653.67	Joback Method
cpg	411.74	J/molxK	686.17	Joback Method
cpg	424.12	J/molxK	718.67	Joback Method
cpg	435.77	J/molxK	751.17	Joback Method
cpg	446.71	J/molxK	783.67	Joback Method
dvisc	0.0073369	Paxs	327.31	Joback Method

dvisc	0.0023928	Paxs	370.87	Joback Method
dvisc	0.0009877	Paxs	414.43	Joback Method
dvisc	0.0004824	Paxs	457.99	Joback Method
dvisc	0.0002668	Paxs	501.55	Joback Method
dvisc	0.0001623	Paxs	545.11	Joback Method
dvisc	0.0001062	Paxs	588.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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

Latest version available from:

<https://www.chemeo.com/cid/49-519-2/2-Hydroxy-cyclohexanecarboxylic-acid-ethyl-ester-trans.pdf>

Generated by Cheméo on 2024-04-30 01:22:52.485834004 +0000 UTC m=+16729421.406411316.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.