2-Hydroxy-cycloheptanecarboxylic acid ethyl ester, cis

Inchi: InChI=1S/C10H18O3/c1-2-13-10(12)8-6-4-3-5-7-9(8)11/h8-9,11H,2-7H2,1H3/t8-,9+/m0/s

InchiKey: ALKWBBFKXDLSML-DTWKUNHWSA-N

Formula: C10H18O3

SMILES: CCOC(=O)C1CCCCCC1O

Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-332.78	kJ/mol	Joback Method
hf	-618.94	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	63.98	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.491		Crippen Method
mcvol	154.210	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1326.00		NIST Webbook
tb	615.82	K	Joback Method
tc	814.37	K	Joback Method
tf	335.06	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.77	J/mol×K	615.82	Joback Method
cpg	437.76	J/mol×K	648.91	Joback Method
cpg	452.88	J/mol×K	682.00	Joback Method
cpg	467.16	J/mol×K	715.10	Joback Method
cpg	480.58	J/mol×K	748.19	Joback Method
cpg	493.15	J/mol×K	781.28	Joback Method
cpg	504.87	J/mol×K	814.37	Joback Method

dvisc	0.0071736	Pa×s	335.06	Joback Method
dvisc	0.0020462	Pa×s	381.85	Joback Method
dvisc	0.0007676	Pa×s	428.65	Joback Method
dvisc	0.0003492	Pa×s	475.44	Joback Method
dvisc	0.0001830	Pa×s	522.23	Joback Method
dvisc	0.0001066	Pa×s	569.03	Joback Method
dvisc	0.0000674	Pa×s	615.82	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=R136660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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