

2-Hydroxy-cycloheptanecarboxylic acid ethyl ester, trans

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-IUCAKERBSA-N
Formula:	C10H18O3
SMILES:	CCOC(=O)C1CCCCC1O
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
mvol	154.210	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	615.82	K	Joback Method
tc	814.37	K	Joback Method
tf	335.06	K	Joback Method
vc	0.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.77	J/molxK	615.82	Joback Method
cpg	493.15	J/molxK	781.28	Joback Method
cpg	480.58	J/molxK	748.19	Joback Method
cpg	467.16	J/molxK	715.10	Joback Method
cpg	452.88	J/molxK	682.00	Joback Method
cpg	437.76	J/molxK	648.91	Joback Method
cpg	504.87	J/molxK	814.37	Joback Method
dvisc	0.0000674	Paxs	615.82	Joback Method

dvisc	0.0001066	Paxs	569.03	Joback Method
dvisc	0.0001830	Paxs	522.23	Joback Method
dvisc	0.0003492	Paxs	475.44	Joback Method
dvisc	0.0007676	Paxs	428.65	Joback Method
dvisc	0.0020462	Paxs	381.85	Joback Method
dvisc	0.0071736	Paxs	335.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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