

4,7-Methanoindan-2,5-dicarboxylic acid, hexahydro-

Inchi:	InChI=1S/C12H16O4/c13-11(14)6-3-7-5-1-9(8(7)4-6)10(2-5)12(15)16/h5-10H,1-4H2,(H,1
InchiKey:	RKLMSTQEVORNHJ-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	O=C(O)C1CC2C3CC(C(=O)O)C(C3)C2C1
Mol. weight [g/mol]:	224.25
CAS:	87324-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-334.30	kJ/mol	Joback Method
hf	-669.41	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	88.14	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.454		Crippen Method
mcvol	162.240	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	776.54	K	Joback Method
tc	975.86	K	Joback Method
tf	484.08	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.78	J/molxK	776.54	Joback Method
cpg	556.12	J/molxK	809.76	Joback Method
cpg	567.72	J/molxK	842.98	Joback Method
cpg	578.66	J/molxK	876.20	Joback Method
cpg	589.01	J/molxK	909.42	Joback Method
cpg	598.83	J/molxK	942.64	Joback Method
cpg	608.20	J/molxK	975.86	Joback Method
dvisc	0.0041564	Paxs	484.08	Joback Method
dvisc	0.0022300	Paxs	532.82	Joback Method

dvisc	0.0013281	Paxs	581.57	Joback Method
dvisc	0.0008570	Paxs	630.31	Joback Method
dvisc	0.0005889	Paxs	679.05	Joback Method
dvisc	0.0004255	Paxs	727.80	Joback Method
dvisc	0.0003202	Paxs	776.54	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=C87324445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	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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