

1,4-Dihydronaphthalene-1,4-dicarboxylic acid

Inchi:	InChI=1S/C12H10O4/c13-11(14)9-5-6-10(12(15)16)8-4-2-1-3-7(8)9/h1-6,9-10H,(H,13,14)
InchiKey:	FMPOSZITAILTAE-UHFFFAOYSA-N
Formula:	C12H10O4
SMILES:	O=C(O)C1C=CC(C(=O)O)c2ccccc21
Mol. weight [g/mol]:	218.21
CAS:	18274-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-307.64	kJ/mol	Joback Method
hf	-491.49	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	92.16	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.593		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	803.22	K	Joback Method
tc	1013.60	K	Joback Method
tf	496.38	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.31	J/molxK	803.22	Joback Method
cpg	456.17	J/molxK	838.28	Joback Method
cpg	464.37	J/molxK	873.35	Joback Method
cpg	471.94	J/molxK	908.41	Joback Method
cpg	478.93	J/molxK	943.48	Joback Method
cpg	485.39	J/molxK	978.54	Joback Method
cpg	491.38	J/molxK	1013.60	Joback Method
dvisc	0.0008836	Paxs	496.38	Joback Method
dvisc	0.0003643	Paxs	547.52	Joback Method

dvisc	0.0001748	Paxs	598.66	Joback Method
dvisc	0.0000941	Paxs	649.80	Joback Method
dvisc	0.0000555	Paxs	700.94	Joback Method
dvisc	0.0000351	Paxs	752.08	Joback Method
dvisc	0.0000236	Paxs	803.22	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=C18274345&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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