

1,4,5,8-Naphthalenetetracarboxylic acid

Other names:	Tetra acid 1,4,5,8-Tetracarboxynaphthalene naphthalene-1,4,5,8-tetracarboxylic acid
Inchi:	InChI=1S/C14H8O8/c15-11(16)5-1-2-6(12(17)18)10-8(14(21)22)4-3-7(9(5)10)13(19)20/h
InchiKey:	OLAPPGSPBNVTRF-UHFFFAOYSA-N
Formula:	C14H8O8
SMILES:	O=C(O)c1ccc(C(=O)O)c2c(C(=O)O)ccc(C(=O)O)c12
Mol. weight [g/mol]:	304.21
CAS:	128-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-815.42	kJ/mol	Joback Method
hf	-1009.81	kJ/mol	Joback Method
hfus	44.27	kJ/mol	Joback Method
hvap	147.02	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	1.633		Crippen Method
mcvol	194.660	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	1169.50	K	Joback Method
tc	1444.42	K	Joback Method
tf	799.74	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	1169.50	Joback Method
cpg	597.18	J/mol×K	1398.60	Joback Method
cpg	592.89	J/mol×K	1352.78	Joback Method
cpg	588.54	J/mol×K	1306.96	Joback Method
cpg	584.05	J/mol×K	1261.14	Joback Method
cpg	579.31	J/mol×K	1215.32	Joback Method

cpg	601.51	J/mol×K	1444.42	Joback Method
dvisc	5.4050678e-08	Pa×s	1169.50	Joback Method
dvisc	8.3019371e-08	Pa×s	1107.87	Joback Method
dvisc	0.0000001	Pa×s	1046.25	Joback Method
dvisc	0.0000002	Pa×s	984.62	Joback Method
dvisc	0.0000004	Pa×s	922.99	Joback Method
dvisc	0.0000009	Pa×s	861.37	Joback Method
dvisc	0.0000019	Pa×s	799.74	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=C128972&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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