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

Physical Properties

Property code	Value	Unit	Source
af	1.3024		Cheméo Relay (1.0)
gf	-815.42	kJ/mol	Joback Method
hf	-1248.76	kJ/mol	Cheméo Relay (1.0)
hfus	44.27	kJ/mol	Joback Method
hvap	171.67	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	1.633		Crippen Method
mcvol	194.660	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	637.49	K	Cheméo Relay (1.0)
tc	1105.97	K	Cheméo Relay (1.0)
tf	569.88	K	Cheméo Relay (1.0)
vc	0.678	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	597.18	J/mol×K	1398.60	Joback Method
cpg	601.51	J/mol×K	1444.42	Joback Method
dvisc	0.0000019	Pa×s	799.74	Joback Method
dvisc	0.0000009	Pa×s	861.37	Joback Method
dvisc	0.0000004	Pa×s	922.99	Joback Method
dvisc	0.0000002	Pa×s	984.62	Joback Method
dvisc	0.0000001	Pa×s	1046.25	Joback Method
dvisc	8.3019371e-08	Pa×s	1107.87	Joback Method
dvisc	5.4050678e-08	Pa×s	1169.50	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128972&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie: Ionization energy
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