

1,6-Naphthalenedicarboxylic acid

Other names:	naphthalene-1,6-dicarboxylic acid
Inchi:	InChI=1S/C12H8O4/c13-11(14)8-4-5-9-7(6-8)2-1-3-10(9)12(15)16/h1-6H,(H,13,14)(H,15)
InchiKey:	VAWFFNJAPKXVPH-UHFFFAOYSA-N
Formula:	C12H8O4
SMILES:	O=C(O)c1ccc2c(C(=O)O)cccc2c1
Mol. weight [g/mol]:	216.19
CAS:	2089-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-281.52	kJ/mol	Joback Method
hf	-415.97	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	94.40	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.236		Crippen Method
mcvol	151.600	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	821.68	K	Joback Method
tc	1035.21	K	Joback Method
tf	530.66	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.62	J/mol×K	821.68	Joback Method
cpg	413.86	J/mol×K	857.27	Joback Method
cpg	420.61	J/mol×K	892.86	Joback Method
cpg	426.90	J/mol×K	928.45	Joback Method
cpg	432.80	J/mol×K	964.03	Joback Method
cpg	438.35	J/mol×K	999.62	Joback Method
cpg	443.61	J/mol×K	1035.21	Joback Method
dvisc	0.0004215	Pa×s	530.66	Joback Method

dvisc	0.0001913	Pa×s	579.16	Joback Method
dvisc	0.0000981	Pa×s	627.67	Joback Method
dvisc	0.0000554	Pa×s	676.17	Joback Method
dvisc	0.0000337	Pa×s	724.67	Joback Method
dvisc	0.0000219	Pa×s	773.18	Joback Method
dvisc	0.0000149	Pa×s	821.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2089874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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