

Naphthalene-1,4,5,8-tetracarboxylic acid, tetramethyl ester

Other names:	1,4,5,8-Tetracarbomethoxynaphthalene
Inchi:	InChI=1S/C18H16O8/c1-23-15(19)9-5-6-11(17(21)25-3)14-12(18(22)26-4)8-7-10(13(9)14)
InchiKey:	QGAXWPQVUFUUSGN-UHFFFAOYSA-N
Formula:	C18H16O8
SMILES:	<chem>COC(=O)c1ccc(C(=O)OC)c2c(C(=O)OC)ccc(C(=O)OC)c12</chem>
Mol. weight [g/mol]:	360.31
CAS:	31996-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-654.46	kJ/mol	Joback Method
hf	-1012.33	kJ/mol	Joback Method
hfus	43.03	kJ/mol	Joback Method
hvap	98.85	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	1.986		Crippen Method
mcvol	251.020	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
tb	981.98	K	Joback Method
tc	1213.81	K	Joback Method
tf	690.46	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.46	J/molxK	981.98	Joback Method
cpg	760.90	J/molxK	1020.62	Joback Method
cpg	767.92	J/molxK	1059.26	Joback Method
cpg	773.51	J/molxK	1097.89	Joback Method
cpg	777.64	J/molxK	1136.53	Joback Method
cpg	780.31	J/molxK	1175.17	Joback Method
cpg	781.50	J/molxK	1213.81	Joback Method
dvisc	0.0002997	Paxs	690.46	Joback Method

dvisc	0.0002250	Paxs	739.05	Joback Method
dvisc	0.0001751	Paxs	787.63	Joback Method
dvisc	0.0001402	Paxs	836.22	Joback Method
dvisc	0.0001151	Paxs	884.81	Joback Method
dvisc	0.0000964	Paxs	933.39	Joback Method
dvisc	0.0000822	Paxs	981.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31996108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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