2,6-Naphthalenedicarboxylic acid, dimethyl ester

Other names: Dimethyl 2,6-naphthalenedicarboxylate
Dimethyl naphthalene-2,6-dicarboxylate
2,6-Dicarbomethoxynaphthalene
Naphthalene-2,6-dicarboxylic acid, dimethyl ester
Dimethyl ester of 2,6-naphthalenedicarboxylic acid

Inchi: InChI=1S/C14H12O4/c1-17-13(15)11-5-3-10-8-12(14(16)18-2)6-4-9(10)7-11/h3-8H,1-2H

InchiKey: GYUVMLBYMPKZAZ-UHFFFAOYSA-N

Formula: C14H12O4

SMILES: COC(=O)c1ccc2cc(C(=O)OC)ccc2c1

Mol. weight [g/mol]: 244.24

CAS: 840-65-3

Physical Properties

Property code	Value	Unit	Source
chs	-6527.60 ± 1.20	kJ/mol	NIST Webbook
gf	-201.04	kJ/mol	Joback Method
hf	-555.10 ± 6.10	kJ/mol	NIST Webbook
hfs	-696.50 ± 1.30	kJ/mol	NIST Webbook
hfus	27.87	kJ/mol	Joback Method
hsub	141.40	kJ/mol	NIST Webbook
hvap	70.31	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.413		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	2118.00		NIST Webbook
tb	727.92	K	Joback Method
tc	957.77	K	Joback Method
tf	464.50 ± 0.70	K	NIST Webbook
tf	464.40 ± 0.10	K	NIST Webbook
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.23	J/mol×K	957.77	Joback Method
cpg	525.12	J/mol×K	919.46	Joback Method
cpg	516.19	J/mol×K	881.15	Joback Method
cpg	506.41	J/mol×K	842.84	Joback Method
cpg	495.76	J/mol×K	804.54	Joback Method
cpg	484.21	J/mol×K	766.23	Joback Method
cpg	471.72	J/mol×K	727.92	Joback Method
cps	283.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0002177	Pa×s	727.92	Joback Method
dvisc	0.0002576	Pa×s	685.94	Joback Method
dvisc	0.0003115	Pa×s	643.95	Joback Method
dvisc	0.0003867	Pa×s	601.97	Joback Method
dvisc	0.0004960	Pa×s	559.99	Joback Method
dvisc	0.0006624	Pa×s	518.00	Joback Method
dvisc	0.0009310	Pa×s	476.02	Joback Method
hfust	53.30	kJ/mol	464.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C840653&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume