1-Naphthoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C18H14O3/c1-20-14-9-11-15(12-10-14)21-18(19)17-8-4-6-13-5-2-3-7-16(13)17
InchiKey: ILRFBNJKBMHNJD-UHFFFAOYSA-N
Formula: C18H14O3
SMILES: COc1ccc(OC(=O)c2cccc3ccccc23)cc1
Mol. weight [g/mol]: 278.30

Physical Properties

Property code	Value	Unit	Source
gf	73.97	kJ/mol	Joback Method
hf	-150.68	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.068		Crippen Method
mcvol	210.810	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	2492.00		NIST Webbook
tb	792.25	K	Joback Method
tc	1040.33	K	Joback Method
tf	497.59	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.92	J/mol×K	792.25	Joback Method
cpg	595.04	J/mol×K	833.60	Joback Method
cpg	607.93	J/mol×K	874.94	Joback Method
cpg	619.64	J/mol×K	916.29	Joback Method
cpg	630.26	J/mol×K	957.64	Joback Method
cpg	639.85	J/mol×K	998.99	Joback Method
cpg	648.48	J/mol×K	1040.33	Joback Method
dvisc	0.0007242	Pa×s	497.59	Joback Method
dvisc	0.0004901	Pa×s	546.70	Joback Method

dvisc	0.0003538	Pa×s	595.81	Joback Method
dvisc	0.0002683	Pa×s	644.92	Joback Method
dvisc	0.0002117	Pa×s	694.03	Joback Method
dvisc	0.0001723	Pa×s	743.14	Joback Method
dvisc	0.0001438	Pa×s	792.25	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=U307826&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume