1-Naphthoic acid, 2-naphthyl ester

Inchi: InChI=1S/C21H14O2/c22-21(20-11-5-9-16-7-3-4-10-19(16)20)23-18-13-12-15-6-1-2-8-17
InchiKey: LBPUSPRZVDFQNG-UHFFFAOYSA-N
Formula: C21H14O2
SMILES: O=C(Oc1ccc2ccccc2c1)c1cccc2ccccc12
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	310.88	kJ/mol	Joback Method
hf	110.69	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	80.65	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	5.212		Crippen Method
mcvol	227.750	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2870.00		NIST Webbook
tb	857.45	K	Joback Method
tc	1120.51	K	Joback Method
tf	541.87	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.39	J/mol×K	857.45	Joback Method
cpg	658.17	J/mol×K	901.29	Joback Method
cpg	670.88	J/mol×K	945.14	Joback Method
cpg	682.71	J/mol×K	988.98	Joback Method
cpg	693.81	J/mol×K	1032.82	Joback Method
cpg	704.37	J/mol×K	1076.67	Joback Method
cpg	714.55	J/mol×K	1120.51	Joback Method
dvisc	0.0010508	Pa×s	541.87	Joback Method
dvisc	0.0007549	Pa×s	594.47	Joback Method

dvisc	0.0005723	Pa×s	647.06	Joback Method
dvisc	0.0004523	Pa×s	699.66	Joback Method
dvisc	0.0003695	Pa×s	752.26	Joback Method
dvisc	0.0003098	Pa×s	804.85	Joback Method
dvisc	0.0002655	Pa×s	857.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307830&Units=SI

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