1-Naphthaleneacetic acid, hept-2-yl ester

Inchi: InChI=1S/C19H24O2/c1-3-4-5-9-15(2)21-19(20)14-17-12-8-11-16-10-6-7-13-18(16)17/h6
InchiKey: WHRWQXSIZHRSRB-UHFFFAOYSA-N
Formula: C19H24O2
SMILES: CCCCCC(C)OC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	82.17	kJ/mol	Joback Method
hf	-269.44	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.894		Crippen Method
mcvol	242.790	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2740.00		NIST Webbook
tb	760.61	K	Joback Method
tc	973.46	K	Joback Method
tf	432.69	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.43	J/mol×K	760.61	Joback Method
cpg	718.16	J/mol×K	796.08	Joback Method
cpg	733.81	J/mol×K	831.56	Joback Method
cpg	748.44	J/mol×K	867.03	Joback Method
cpg	762.11	J/mol×K	902.51	Joback Method
cpg	774.89	J/mol×K	937.98	Joback Method
cpg	786.83	J/mol×K	973.46	Joback Method
dvisc	0.0012942	Pa×s	432.69	Joback Method
dvisc	0.0007336	Pa×s	487.34	Joback Method

dvisc	0.0004663	Pa×s	542.00	Joback Method
dvisc	0.0003220	Pa×s	596.65	Joback Method
dvisc	0.0002367	Pa×s	651.30	Joback Method
dvisc	0.0001824	Pa×s	705.96	Joback Method
dvisc	0.0001460	Pa×s	760.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415047&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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