1-naphthaleneacetic acid, heptyl ester

Inchi: InChI=1S/C19H24O2/c1-2-3-4-5-8-14-21-19(20)15-17-12-9-11-16-10-6-7-13-18(16)17/h6
InchiKey: AQOHGCUPDSXLGK-UHFFFAOYSA-N
Formula: C19H24O2
SMILES: CCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]: 284.39
CAS: 2876-72-4

Physical Properties

Property code	Value	Unit	Source
af	0.7962		Cheméo Relay (1.0)
hf	-361.30	kJ/mol	Cheméo Relay (1.0)
hfus	38.42	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-5.38		Cheméo Relay (1.0)
logp	4.896		Crippen Method
mcvol	242.790	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
tb	655.28	K	Cheméo Relay (1.0)
tc	882.26	K	Cheméo Relay (1.0)
tf	307.34	K	Cheméo Relay (1.0)
vc	0.902	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.90	J/mol×K	761.05	Joback Method
cpg	717.36	J/mol×K	795.99	Joback Method
cpg	732.80	J/mol×K	830.92	Joback Method
cpg	747.25	J/mol×K	865.86	Joback Method
cpg	760.78	J/mol×K	900.80	Joback Method
cpg	773.46	J/mol×K	935.73	Joback Method
cpg	785.33	J/mol×K	970.67	Joback Method
dvisc	0.0011478	Pa×s	447.69	Joback Method

dvisc	0.0006946	Pa×s	499.92	Joback Method
dvisc	0.0004622	Pa×s	552.14	Joback Method
dvisc	0.0003300	Pa×s	604.37	Joback Method
dvisc	0.0002486	Pa×s	656.60	Joback Method
dvisc	0.0001953	Pa×s	708.82	Joback Method
dvisc	0.0001585	Pa×s	761.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876724&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	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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