Octanoic acid, 2-naphthyl ester

Other names: Octanoic acid, 2-naphthalenyl ester
Octanoic acid, 2-naphthyl ester
Inchi: InChI=1S/C18H22O2/c1-2-3-4-5-6-11-18(19)20-17-13-12-15-9-7-8-10-16(15)14-17/h7-10
InchiKey: CXVZBUOSDMLXNK-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: CCCCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
af	0.8017		Cheméo Relay (1.0)
hf	-343.19	kJ/mol	Cheméo Relay (1.0)
hfus	35.83	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Cheméo Relay (1.0)
ie	7.88	eV	Cheméo Relay (1.0)
log10ws	-5.85		Cheméo Relay (1.0)
logp	5.106		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	640.02	K	Cheméo Relay (1.0)
tc	879.23	K	Cheméo Relay (1.0)
tf	328.98	K	Cheméo Relay (1.0)
vc	0.851	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.16	J/mol×K	738.17	Joback Method
cpg	661.36	J/mol×K	773.51	Joback Method
cpg	676.53	J/mol×K	808.85	Joback Method
cpg	690.72	J/mol×K	844.19	Joback Method
cpg	703.99	J/mol×K	879.53	Joback Method

cpg	716.40	J/mol×K	914.87	Joback Method
cpg	728.02	J/mol×K	950.21	Joback Method
dvisc	0.0012149	Pa×s	436.42	Joback Method
dvisc	0.0007463	Pa×s	486.71	Joback Method
dvisc	0.0005022	Pa×s	537.00	Joback Method
dvisc	0.0003617	Pa×s	587.29	Joback Method
dvisc	0.0002744	Pa×s	637.59	Joback Method
dvisc	0.0002167	Pa×s	687.88	Joback Method
dvisc	0.0001767	Pa×s	738.17	Joback Method

Sources

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=C10251179&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume