

1-Naphthaleneacetic acid, octyl ester

Inchi:	InChI=1S/C20H26O2/c1-2-3-4-5-6-9-15-22-20(21)16-18-13-10-12-17-11-7-8-14-19(17)18
InchiKey:	CZANVDHOSUAOQW-UHFFFAOYSA-N
Formula:	C20H26O2
SMILES:	CCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	93.03	kJ/mol	Joback Method
hf	-284.80	kJ/mol	Joback Method
hfus	41.01	kJ/mol	Joback Method
hvap	73.85	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.286		Crippen Method
mcvol	256.880	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	783.93	K	Joback Method
tc	991.65	K	Joback Method
tf	458.96	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.67	J/mol×K	783.93	Joback Method
cpg	831.40	J/mol×K	957.03	Joback Method
cpg	818.49	J/mol×K	922.41	Joback Method
cpg	804.73	J/mol×K	887.79	Joback Method
cpg	790.04	J/mol×K	853.17	Joback Method
cpg	774.38	J/mol×K	818.55	Joback Method
cpg	843.51	J/mol×K	991.65	Joback Method
dvisc	0.0001416	Pa×s	783.93	Joback Method

dvisc	0.0001751	Pa×s	729.77	Joback Method
dvisc	0.0002241	Pa×s	675.61	Joback Method
dvisc	0.0002995	Pa×s	621.44	Joback Method
dvisc	0.0004229	Pa×s	567.28	Joback Method
dvisc	0.0006424	Pa×s	513.12	Joback Method
dvisc	0.0010769	Pa×s	458.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394009&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

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