

1-Naphthaleneacetic acid, 2-ethylhexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	90.59	kJ/mol	Joback Method
hf	-290.08	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	73.46	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.142		Crippen Method
mvol	256.880	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2719.00		NIST Webbook
tb	783.49	K	Joback Method
tc	994.14	K	Joback Method
tf	443.96	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.20	J/molxK	783.49	Joback Method
cpg	832.73	J/molxK	959.03	Joback Method
cpg	819.74	J/molxK	923.92	Joback Method
cpg	805.85	J/molxK	888.81	Joback Method
cpg	791.01	J/molxK	853.71	Joback Method
cpg	775.14	J/molxK	818.60	Joback Method
cpg	844.90	J/molxK	994.14	Joback Method
dvisc	0.0001301	Paxs	783.49	Joback Method
dvisc	0.0001633	Paxs	726.90	Joback Method

dvisc	0.0002129	Paxs	670.31	Joback Method
dvisc	0.0002915	Paxs	613.73	Joback Method
dvisc	0.0004255	Paxs	557.14	Joback Method
dvisc	0.0006763	Paxs	500.55	Joback Method
dvisc	0.0012100	Paxs	443.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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