

1-Naphthaleneacetic acid, decyl ester

Inchi:	InChI=1S/C22H30O2/c1-2-3-4-5-6-7-8-11-17-24-22(23)18-20-15-12-14-19-13-9-10-16-2
InchiKey:	QSZJDPRXGPPFIR-UHFFFAOYSA-N
Formula:	C22H30O2
SMILES:	CCCCCCCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	109.87	kJ/mol	Joback Method
hf	-326.08	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.066		Crippen Method
mvol	285.060	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	829.69	K	Joback Method
tc	1035.36	K	Joback Method
tf	481.50	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.05	J/molxK	829.69	Joback Method
cpg	949.91	J/molxK	1001.08	Joback Method
cpg	936.58	J/molxK	966.80	Joback Method
cpg	922.40	J/molxK	932.52	Joback Method
cpg	907.29	J/molxK	898.25	Joback Method
cpg	891.20	J/molxK	863.97	Joback Method
cpg	962.44	J/molxK	1035.36	Joback Method
dvisc	0.0001114	Paxs	829.69	Joback Method

dvisc	0.0001390	Paxs	771.66	Joback Method
dvisc	0.0001796	Paxs	713.63	Joback Method
dvisc	0.0002429	Paxs	655.60	Joback Method
dvisc	0.0003484	Paxs	597.56	Joback Method
dvisc	0.0005401	Paxs	539.53	Joback Method
dvisc	0.0009304	Paxs	481.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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