

1-Naphthaleneacetic acid, butyl ester

Inchi:	InChI=1S/C16H18O2/c1-2-3-11-18-16(17)12-14-9-6-8-13-7-4-5-10-15(13)14/h4-10H,2-3,
InchiKey:	ONFNCARYSQWBPI-UHFFFAOYSA-N
Formula:	C16H18O2
SMILES:	CCCCOC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	59.35	kJ/mol	Joback Method
hf	-202.24	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.726		Crippen Method
mvol	200.520	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1979.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	692.41	K	Joback Method
tc	910.70	K	Joback Method
tf	413.88	K	Joback Method
vc	0.769	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.07	J/molxK	692.41	Joback Method
cpg	552.60	J/molxK	728.79	Joback Method
cpg	567.11	J/molxK	765.17	Joback Method
cpg	580.65	J/molxK	801.56	Joback Method
cpg	593.27	J/molxK	837.94	Joback Method
cpg	605.05	J/molxK	874.32	Joback Method
cpg	616.03	J/molxK	910.70	Joback Method
dvisc	0.0013297	Paxs	413.88	Joback Method

dvisc	0.0008431	Paxs	460.30	Joback Method
dvisc	0.0005811	Paxs	506.72	Joback Method
dvisc	0.0004263	Paxs	553.14	Joback Method
dvisc	0.0003282	Paxs	599.57	Joback Method
dvisc	0.0002623	Paxs	645.99	Joback Method
dvisc	0.0002160	Paxs	692.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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