

1-Naphthaleneacetic acid, isobutyl ester

Inchi:	InChI=1S/C16H18O2/c1-12(2)11-18-16(17)10-14-8-5-7-13-6-3-4-9-15(13)14/h3-9,12H,10
InchiKey:	AQLLHLGWSOYTKT-UHFFFAOYSA-N
Formula:	C16H18O2
SMILES:	CC(C)COC(=O)Cc1cccc2ccccc12
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	56.91	kJ/mol	Joback Method
hf	-207.52	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.581		Crippen Method
mvol	200.520	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	691.97	K	Joback Method
tc	914.36	K	Joback Method
tf	398.88	K	Joback Method
vc	0.763	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.59	J/molxK	691.97	Joback Method
cpg	553.44	J/molxK	729.03	Joback Method
cpg	568.21	J/molxK	766.10	Joback Method
cpg	581.97	J/molxK	803.16	Joback Method
cpg	594.78	J/molxK	840.23	Joback Method
cpg	606.69	J/molxK	877.29	Joback Method
cpg	617.76	J/molxK	914.36	Joback Method
dvisc	0.0015154	Paxs	398.88	Joback Method

dvisc	0.0008993	Paxs	447.73	Joback Method
dvisc	0.0005914	Paxs	496.58	Joback Method
dvisc	0.0004192	Paxs	545.42	Joback Method
dvisc	0.0003145	Paxs	594.27	Joback Method
dvisc	0.0002464	Paxs	643.12	Joback Method
dvisc	0.0001999	Paxs	691.97	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=U393977&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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