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
CAS: 2876-75-7

Physical Properties

Property code	Value	Unit	Source
af	0.6687		Cheméo Relay (1.0)
hf	-299.79	kJ/mol	Cheméo Relay (1.0)
hfus	30.65	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Cheméo Relay (1.0)
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	3.726		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
tb	622.68	K	Cheméo Relay (1.0)
tc	854.10	K	Cheméo Relay (1.0)
tf	294.28	K	Cheméo Relay (1.0)
vc	0.737	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0008431	Pa×s	460.30	Joback Method
dvisc	0.0005811	Pa×s	506.72	Joback Method
dvisc	0.0004263	Pa×s	553.14	Joback Method
dvisc	0.0003282	Pa×s	599.57	Joback Method
dvisc	0.0002623	Pa×s	645.99	Joback Method
dvisc	0.0002160	Pa×s	692.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876757&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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