

1-Naphthaleneacetic acid, cyclohexylmethyl ester

Inchi:	InChI=1S/C19H22O2/c20-19(21-14-15-7-2-1-3-8-15)13-17-11-6-10-16-9-4-5-12-18(16)1
InchiKey:	PGDITAURKHRFTK-UHFFFAOYSA-N
Formula:	C19H22O2
SMILES:	O=C(Cc1cccc2ccccc12)OCC1CCCCC1
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	109.06	kJ/mol	Joback Method
hf	-209.84	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.506		Crippen Method
mcvol	231.930	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinsol	2825.00		NIST Webbook
tb	780.60	K	Joback Method
tc	1020.26	K	Joback Method
tf	455.07	K	Joback Method
vc	0.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.14	J/molxK	780.60	Joback Method
cpg	773.75	J/molxK	980.32	Joback Method
cpg	760.63	J/molxK	940.38	Joback Method
cpg	746.30	J/molxK	900.43	Joback Method
cpg	730.67	J/molxK	860.49	Joback Method
cpg	713.65	J/molxK	820.54	Joback Method
cpg	785.76	J/molxK	1020.26	Joback Method
dvisc	0.0001677	Paxs	780.60	Joback Method
dvisc	0.0002085	Paxs	726.35	Joback Method

dvisc	0.0002686	Paxs	672.09	Joback Method
dvisc	0.0003616	Paxs	617.84	Joback Method
dvisc	0.0005156	Paxs	563.58	Joback Method
dvisc	0.0007929	Paxs	509.32	Joback Method
dvisc	0.0013510	Paxs	455.07	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=U415049&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
mccvol:	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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