

1-Naphthaleneacetic acid, naphth-2-ylmethyl ester

Inchi:	InChI=1S/C23H18O2/c24-23(15-21-10-5-9-19-7-3-4-11-22(19)21)25-16-17-12-13-18-6-1
InchiKey:	RKVHWVCZDFXDSZ-UHFFFAOYSA-N
Formula:	C23H18O2
SMILES:	O=C(Cc1cccc2ccccc12)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	327.72	kJ/mol	Joback Method
hf	69.41	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	85.10	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.279		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinsol	1664.00		NIST Webbook
tb	903.21	K	Joback Method
tc	1156.52	K	Joback Method
tf	564.41	K	Joback Method
vc	0.976	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.31	J/molxK	903.21	Joback Method
cpg	820.86	J/molxK	1114.30	Joback Method
cpg	809.44	J/molxK	1072.08	Joback Method
cpg	797.54	J/molxK	1029.87	Joback Method
cpg	784.99	J/molxK	987.65	Joback Method
cpg	771.64	J/molxK	945.43	Joback Method
cpg	831.96	J/molxK	1156.52	Joback Method
dvisc	0.0002132	Paxs	903.21	Joback Method
dvisc	0.0002511	Paxs	846.74	Joback Method

dvisc	0.0003027	Paxs	790.28	Joback Method
dvisc	0.0003755	Paxs	733.81	Joback Method
dvisc	0.0004828	Paxs	677.34	Joback Method
dvisc	0.0006500	Paxs	620.88	Joback Method
dvisc	0.0009285	Paxs	564.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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