

2-NAPHTHYLPROPIONIC ACID

Other names:	2-(1-Naphthyl)propionic acid
Inchi:	InChI=1S/C13H12O2/c1-9(13(14)15)11-8-4-6-10-5-2-3-7-12(10)11/h2-9H,1H3,(H,14,15)
InchiKey:	VKCNNDPZFOVURD-UHFFFAOYSA-N
Formula:	C13H12O2
SMILES:	CC(C(=O)O)c1cccc2ccccc12
Mol. weight [g/mol]:	200.24

Physical Properties

Property code	Value	Unit	Source
hf	-290.65	kJ/mol	Cheméo Relay (1.0)
hfus	22.26	kJ/mol	Joback Method
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	3.028		Crippen Method
mcvol	158.250	ml/mol	McGowan Method
rinpol	1984.00		NIST Webbook
tb	605.83	K	Cheméo Relay (1.0)
tf	378.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.52	J/mol×K	693.09	Joback Method
cpg	422.01	J/mol×K	729.69	Joback Method
cpg	432.68	J/mol×K	766.29	Joback Method
cpg	442.60	J/mol×K	802.89	Joback Method
cpg	451.84	J/mol×K	839.49	Joback Method
cpg	460.45	J/mol×K	876.08	Joback Method
cpg	468.51	J/mol×K	912.68	Joback Method
dvisc	0.0023917	Pa×s	403.66	Joback Method
dvisc	0.0010200	Pa×s	451.90	Joback Method
dvisc	0.0005127	Pa×s	500.14	Joback Method
dvisc	0.0002909	Pa×s	548.38	Joback Method
dvisc	0.0001809	Pa×s	596.61	Joback Method

dvisc	0.0001207	Pa×s	644.85	Joback Method
dvisc	0.0000853	Pa×s	693.09	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U129241&Units=SI>

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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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