

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]:	200.23

Physical Properties

Property code	Value	Unit	Source
gf	-0.17	kJ/mol	Joback Method
hf	-165.61	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	72.15	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.028		Crippen Method
mvol	158.250	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1984.00		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	693.09	K	Joback Method
tc	912.68	K	Joback Method
tf	403.66	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.52	J/molxK	693.09	Joback Method
cpg	460.45	J/molxK	876.08	Joback Method
cpg	451.84	J/molxK	839.49	Joback Method
cpg	442.60	J/molxK	802.89	Joback Method
cpg	432.68	J/molxK	766.29	Joback Method
cpg	422.01	J/molxK	729.69	Joback Method
cpg	468.51	J/molxK	912.68	Joback Method

dvisc	0.0000853	Paxs	693.09	Joback Method
dvisc	0.0001207	Paxs	644.85	Joback Method
dvisc	0.0001809	Paxs	596.61	Joback Method
dvisc	0.0002909	Paxs	548.38	Joback Method
dvisc	0.0005127	Paxs	500.14	Joback Method
dvisc	0.0010200	Paxs	451.90	Joback Method
dvisc	0.0023917	Paxs	403.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U129241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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