

1-Naphthalenecarboxamide, N-(4-fluorophenyl)-

Inchi:	InChI=1S/C17H12FNO/c18-13-8-10-14(11-9-13)19-17(20)16-7-3-5-12-4-1-2-6-15(12)16/
InchiKey:	VECQBWJBOOWSSS-UHFFFAOYSA-N
Formula:	C17H12FNO
SMILES:	O=C(Nc1ccc(F)cc1)c1cccc2ccccc12
Mol. weight [g/mol]:	265.28

Physical Properties

Property code	Value	Unit	Source
gf	170.13	kJ/mol	Joback Method
hf	-8.24	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.231		Crippen Method
mcvol	196.730	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	2428.00		NIST Webbook
tb	773.97	K	Joback Method
tc	1020.87	K	Joback Method
tf	495.11	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.87	J/molxK	773.97	Joback Method
cpg	548.08	J/molxK	815.12	Joback Method
cpg	560.17	J/molxK	856.27	Joback Method
cpg	571.28	J/molxK	897.42	Joback Method
cpg	581.52	J/molxK	938.57	Joback Method
cpg	591.01	J/molxK	979.72	Joback Method
cpg	599.86	J/molxK	1020.87	Joback Method

Sources

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=U307404&Units=SI
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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