

Benzamide, n-(1-naphthyl)-3-fluoro-

Inchi:	InChI=1S/C17H12FNO/c18-14-8-3-7-13(11-14)17(20)19-16-10-4-6-12-5-1-2-9-15(12)16/
InchiKey:	BZSXIVIFGVRLJR-UHFFFAOYSA-N
Formula:	C17H12FNO
SMILES:	O=C(Nc1cccc2ccccc12)c1cccc(F)c1
Mol. weight [g/mol]:	265.29

Physical Properties

Property code	Value	Unit	Source
hfus	33.89	kJ/mol	Joback Method
ie	8.01	eV	Cheméo Relay (1.0)
logp	4.231		Crippen Method
mcvol	196.730	ml/mol	McGowan Method
rinpol	2424.00		NIST Webbook
tb	670.00	K	Cheméo Relay (1.0)
tf	422.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307171&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/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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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