

Benzamide, 2,6-difluoro-N-(1-naphthyl)-

Other names:	Benzamide, N-(1-naphthyl)-2,6-difluoro-
Inchi:	InChI=1S/C17H11F2NO/c18-13-8-4-9-14(19)16(13)17(21)20-15-10-3-6-11-5-1-2-7-12(11)
InchiKey:	SZZRVHTXVVVMLC-UHFFFAOYSA-N
Formula:	C17H11F2NO
SMILES:	O=C(Nc1cccc2ccccc12)c1c(F)cccc1F
Mol. weight [g/mol]:	283.27
CAS:	294852-77-0

Physical Properties

Property code	Value	Unit	Source
gf	-34.31	kJ/mol	Joback Method
hf	-215.82	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.370		Crippen Method
mcvol	198.500	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	778.22	K	Joback Method
tc	1015.71	K	Joback Method
tf	508.22	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.13	J/molxK	778.22	Joback Method
cpg	553.59	J/molxK	817.80	Joback Method
cpg	565.04	J/molxK	857.38	Joback Method
cpg	575.59	J/molxK	896.97	Joback Method
cpg	585.32	J/molxK	936.55	Joback Method
cpg	594.34	J/molxK	976.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C294852770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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