

Benzamide, N-decyl-N-methyl-2,6-difluoro-

Inchi:	InChI=1S/C18H27F2NO/c1-3-4-5-6-7-8-9-10-14-21(2)18(22)17-15(19)12-11-13-16(17)20
InchiKey:	OKDMJFWFUQYAFN-UHFFFAOYSA-N
Formula:	C18H27F2NO
SMILES:	CCCCCCCCCN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	311.41

Physical Properties

Property code	Value	Unit	Source
gf	-213.93	kJ/mol	Joback Method
hf	-638.53	kJ/mol	Joback Method
hfus	46.42	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.178		Crippen Method
mvol	255.810	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	712.73	K	Joback Method
tc	893.91	K	Joback Method
tf	427.66	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.29	J/molxK	712.73	Joback Method
cpg	754.11	J/molxK	742.93	Joback Method
cpg	770.03	J/molxK	773.12	Joback Method
cpg	785.08	J/molxK	803.32	Joback Method
cpg	799.31	J/molxK	833.52	Joback Method
cpg	812.75	J/molxK	863.71	Joback Method
cpg	825.44	J/molxK	893.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308667&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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