

Benzamide, 3,4-difluoro-N-nonyl-

Inchi:	InChI=1S/C16H23F2NO/c1-2-3-4-5-6-7-8-11-19-16(20)13-9-10-14(17)15(18)12-13/h9-10
InchiKey:	QDBOWAMYIGFRTF-UHFFFAOYSA-N
Formula:	C16H23F2NO
SMILES:	CCCCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	283.36

Physical Properties

Property code	Value	Unit	Source
gf	-252.16	kJ/mol	Joback Method
hf	-611.31	kJ/mol	Joback Method
hfus	43.32	kJ/mol	Joback Method
hvap	66.36	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.445		Crippen Method
mvol	227.630	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2142.00		NIST Webbook
rinpol	2142.00		NIST Webbook
tb	704.70	K	Joback Method
tc	890.67	K	Joback Method
tf	425.31	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.51	J/mol×K	704.70	Joback Method
cpg	659.91	J/mol×K	735.69	Joback Method
cpg	674.48	J/mol×K	766.69	Joback Method
cpg	688.23	J/mol×K	797.68	Joback Method
cpg	701.20	J/mol×K	828.68	Joback Method
cpg	713.43	J/mol×K	859.67	Joback Method
cpg	724.94	J/mol×K	890.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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