Benzamide, 3,4-difluoro-N-ethyl-

Inchi: InChI=1S/C9H9F2NO/c1-2-12-9(13)6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3,(H,12,13)
InchiKey: ZOTHBTVQULJABH-UHFFFAOYSA-N
Formula: C9H9F2NO
SMILES: CCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 185.17

Physical Properties

Property code	Value	Unit	Source
gf	-311.10	kJ/mol	Joback Method
hf	-466.83	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	50.78	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.715		Crippen Method
mcvol	129.000	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	544.54	K	Joback Method
tc	744.55	K	Joback Method
tf	346.42	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.13	J/mol×K	544.54	Joback Method
cpg	305.28	J/mol×K	577.88	Joback Method
cpg	315.81	J/mol×K	611.21	Joback Method
cpg	325.75	J/mol×K	644.55	Joback Method
cpg	335.09	J/mol×K	677.88	Joback Method
cpg	343.88	J/mol×K	711.22	Joback Method
cpg	352.11	J/mol×K	744.55	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=U407787&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
mcvol:	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