Benzamide, 3,4-difluoro-N-methyl-

Inchi: InChI=1S/C8H7F2NO/c1-11-8(12)5-2-3-6(9)7(10)4-5/h2-4H,1H3,(H,11,12)
InchiKey: HQBRGWPNIBPNHR-UHFFFAOYSA-N
Formula: C8H7F2NO
SMILES: CNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 171.14

Physical Properties

Property code	Value	Unit	Source
gf	-319.52	kJ/mol	Joback Method
hf	-446.19	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.324		Crippen Method
mcvol	114.910	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
tb	521.66	K	Joback Method
tc	724.57	K	Joback Method
tf	335.15	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.57	J/mol×K	521.66	Joback Method
cpg	260.74	J/mol×K	555.48	Joback Method
cpg	270.34	J/mol×K	589.30	Joback Method
cpg	279.38	J/mol×K	623.11	Joback Method
cpg	287.89	J/mol×K	656.93	Joback Method
cpg	295.87	J/mol×K	690.75	Joback Method
cpg	303.35	J/mol×K	724.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U407786&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume