Benzamide, 2,6-difluoro-3-methyl-N-ethyl-

Inchi: InChI=1S/C10H11F2NO/c1-3-13-10(14)8-7(11)5-4-6(2)9(8)12/h4-5H,3H2,1-2H3,(H,13,14
InchiKey: JMAOLOBHOJLICX-UHFFFAOYSA-N
Formula: C10H11F2NO
SMILES: CCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 199.20

Physical Properties

Property code	Value	Unit	Source
gf	-312.31	kJ/mol	Joback Method
hf	-498.94	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.023		Crippen Method
mcvol	143.090	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	572.40	K	Joback Method
tc	770.63	K	Joback Method
tf	370.21	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.92	J/mol×K	572.40	Joback Method
cpg	350.68	J/mol×K	605.44	Joback Method
cpg	361.82	J/mol×K	638.48	Joback Method
cpg	372.36	J/mol×K	671.52	Joback Method
cpg	382.31	J/mol×K	704.55	Joback Method
cpg	391.69	J/mol×K	737.59	Joback Method
cpg	400.51	J/mol×K	770.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407734&Units=SI
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

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