Benzamide, 6-trifluoromethyl-2-fluoro-N-ethyl-

Inchi: InChI=1S/C10H9F4NO/c1-2-15-9(16)8-6(10(12,13)14)4-3-5-7(8)11/h3-5H,2H2,1H3,(H,15
InchiKey: CBLDTECEAYJZQH-UHFFFAOYSA-N
Formula: C10H9F4NO
SMILES: CCNC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 235.18

Physical Properties

Property code	Value	Unit	Source
gf	-689.46	kJ/mol	Joback Method
hf	-888.44	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.594		Crippen Method
mcvol	146.630	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1401.00		NIST Webbook
rinpol	1401.00		NIST Webbook
tb	562.73	K	Joback Method
tc	752.89	K	Joback Method
tf	361.29	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.53	J/mol×K	562.73	Joback Method
cpg	371.10	J/mol×K	594.42	Joback Method
cpg	381.94	J/mol×K	626.12	Joback Method
cpg	392.07	J/mol×K	657.81	Joback Method
cpg	401.54	J/mol×K	689.50	Joback Method
cpg	410.38	J/mol×K	721.20	Joback Method
cpg	418.63	J/mol×K	752.89	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=U407770&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