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

Inchi: InChI=1S/C11H11F4NO/c1-2-6-16-10(17)9-7(11(13,14)15)4-3-5-8(9)12/h3-5H,2,6H2,1H3

InchiKey: MZZMFZZJJPEANR-UHFFFAOYSA-N

Formula: C11H11F4NO

SMILES: CCCNC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 249.20

Physical Properties

Property code	Value	Unit	Source
gf	-681.04	kJ/mol	Joback Method
hf	-909.08	kJ/mol	Joback Method
hfus	29.11	kJ/mol	Joback Method
hvap	52.30	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	2.984		Crippen Method
mcvol	160.720	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	585.61	K	Joback Method
tc	773.57	K	Joback Method
tf	372.56	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.42	J/mol×K	585.61	Joback Method
cpg	418.66	J/mol×K	616.94	Joback Method
cpg	430.15	J/mol×K	648.26	Joback Method
cpg	440.91	J/mol×K	679.59	Joback Method
cpg	450.99	J/mol×K	710.91	Joback Method
cpg	460.42	J/mol×K	742.24	Joback Method
cpg	469.23	J/mol×K	773.57	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=U407771&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

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