Benzamide, 2,3,4-trifluoro-N-propyl-

Inchi: InChI=1S/C10H10F3NO/c1-2-5-14-10(15)6-3-4-7(11)9(13)8(6)12/h3-4H,2,5H2,1H3,(H,14
InchiKey: LWDNRGYDAIXNPR-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: CCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 217.19

Physical Properties

Property code	Value	Unit	Source
gf	-507.12	kJ/mol	Joback Method
hf	-695.05	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.244		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
tb	571.67	K	Joback Method
tc	761.04	K	Joback Method
tf	370.80	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.16	J/mol×K	571.67	Joback Method
cpg	358.37	J/mol×K	603.23	Joback Method
cpg	369.00	J/mol×K	634.79	Joback Method
cpg	379.07	J/mol×K	666.36	Joback Method
cpg	388.58	J/mol×K	697.92	Joback Method
cpg	397.57	J/mol×K	729.48	Joback Method
cpg	406.03	J/mol×K	761.04	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=U407258&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