Benzamide, 3-(trifluoromethyl)-N-propyl-

Inchi: InChI=1S/C11H12F3NO/c1-2-6-15-10(16)8-4-3-5-9(7-8)11(12,13)14/h3-5,7H,2,6H2,1H3,
InchiKey: OPQNVKBIBGFOCD-UHFFFAOYSA-N
Formula: C11H12F3NO
SMILES: CCCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 231.21

Physical Properties

Property code	Value	Unit	Source
gf	-476.60	kJ/mol	Joback Method
hf	-701.50	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.845		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	581.36	K	Joback Method
tc	776.89	K	Joback Method
tf	359.45	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.71	J/mol×K	581.36	Joback Method
cpg	411.80	J/mol×K	613.95	Joback Method
cpg	424.03	J/mol×K	646.54	Joback Method
cpg	435.45	J/mol×K	679.12	Joback Method
cpg	446.10	J/mol×K	711.71	Joback Method
cpg	456.03	J/mol×K	744.30	Joback Method
cpg	465.29	J/mol×K	776.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407165&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