Benzamide, 2-(trifluoromethyl)-N-pentyl-

Inchi: InChI=1S/C13H16F3NO/c1-2-3-6-9-17-12(18)10-7-4-5-8-11(10)13(14,15)16/h4-5,7-8H,2-
InchiKey: DJXYKGOYQXUTLV-UHFFFAOYSA-N
Formula: C13H16F3NO
SMILES: CCCCCNC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 259.27

Physical Properties

Property code	Value	Unit	Source
gf	-459.76	kJ/mol	Joback Method
hf	-742.78	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	56.91	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.625		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	627.12	K	Joback Method
tc	817.97	K	Joback Method
tf	381.99	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.26	J/mol×K	627.12	Joback Method
cpg	511.41	J/mol×K	658.93	Joback Method
cpg	524.69	J/mol×K	690.74	Joback Method
cpg	537.13	J/mol×K	722.55	Joback Method
cpg	548.77	J/mol×K	754.36	Joback Method
cpg	559.68	J/mol×K	786.16	Joback Method
cpg	569.88	J/mol×K	817.97	Joback Method

Sources

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=U407188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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