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

Inchi: InChI=1S/C14H18F3NO/c1-2-3-4-7-10-18-13(19)11-8-5-6-9-12(11)14(15,16)17/h5-6,8-9H
InchiKey: YKPLXBUFLPBXDD-UHFFFAOYSA-N
Formula: C14H18F3NO
SMILES: CCCCCCNC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	-451.34	kJ/mol	Joback Method
hf	-763.42	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.016		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	650.00	K	Joback Method
tc	838.95	K	Joback Method
tf	393.26	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.66	J/mol×K	650.00	Joback Method
cpg	563.25	J/mol×K	681.49	Joback Method
cpg	576.95	J/mol×K	712.98	Joback Method
cpg	589.81	J/mol×K	744.47	Joback Method
cpg	601.87	J/mol×K	775.96	Joback Method
cpg	613.18	J/mol×K	807.46	Joback Method
cpg	623.77	J/mol×K	838.95	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=U407190&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