Benzamide, 3-fluoro-4-trifluoromethyl-N-hexyl-

Inchi: InChI=1S/C14H17F4NO/c1-2-3-4-5-8-19-13(20)10-6-7-11(12(15)9-10)14(16,17)18/h6-7,9
InchiKey: NEDOPJDXZJZBOE-UHFFFAOYSA-N
Formula: C14H17F4NO
SMILES: CCCCCCNC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 291.28

Physical Properties

Property code	Value	Unit	Source
gf	-655.78	kJ/mol	Joback Method
hf	-971.00	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	58.98	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.155		Crippen Method
mcvol	202.990	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	654.25	K	Joback Method
tc	837.13	K	Joback Method
tf	406.37	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.13	J/mol×K	654.25	Joback Method
cpg	569.98	J/mol×K	684.73	Joback Method
cpg	583.01	J/mol×K	715.21	Joback Method
cpg	595.27	J/mol×K	745.69	Joback Method
cpg	606.80	J/mol×K	776.17	Joback Method
cpg	617.63	J/mol×K	806.65	Joback Method
cpg	627.81	J/mol×K	837.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407890&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