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

Inchi: InChI=1S/C13H16F3NO/c1-2-3-4-5-8-17-13(18)9-6-7-10(14)12(16)11(9)15/h6-7H,2-5,8H
InchiKey: USAUDSCIWVILMD-UHFFFAOYSA-N
Formula: C13H16F3NO
SMILES: CCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 259.27

Physical Properties

Property code	Value	Unit	Source
gf	-481.86	kJ/mol	Joback Method
hf	-756.97	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	59.53	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.414		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	640.31	K	Joback Method
tc	824.07	K	Joback Method
tf	404.61	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.02	J/mol×K	640.31	Joback Method
cpg	506.29	J/mol×K	670.94	Joback Method
cpg	518.87	J/mol×K	701.56	Joback Method
cpg	530.78	J/mol×K	732.19	Joback Method
cpg	542.05	J/mol×K	762.82	Joback Method
cpg	552.68	J/mol×K	793.45	Joback Method
cpg	562.71	J/mol×K	824.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407264&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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