Benzamide, 2,3,4-trifluoro-N-butyl-N-octyl-

Inchi: InChI=1S/C19H28F3NO/c1-3-5-7-8-9-10-14-23(13-6-4-2)19(24)15-11-12-16(20)18(22)17
InchiKey: KAPIEOLHFXTNTD-UHFFFAOYSA-N
Formula: C19H28F3NO
SMILES: CCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 343.43

Physical Properties

Property code	Value	Unit	Source
gf	-409.95	kJ/mol	Joback Method
hf	-866.75	kJ/mol	Joback Method
hfus	51.70	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.707		Crippen Method
mcvol	271.670	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	739.86	K	Joback Method
tc	917.83	K	Joback Method
tf	452.04	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.86	J/mol×K	739.86	Joback Method
cpg	818.46	J/mol×K	769.52	Joback Method
cpg	834.17	J/mol×K	799.18	Joback Method
cpg	849.05	J/mol×K	828.85	Joback Method
cpg	863.13	J/mol×K	858.51	Joback Method
cpg	876.42	J/mol×K	888.17	Joback Method
cpg	888.98	J/mol×K	917.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415685&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