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

Inchi: InChI=1S/C16H22F3NO/c1-3-5-7-11-20(10-6-4-2)16(21)12-8-9-13(17)15(19)14(12)18/h8
InchiKey: LPWCPKZARWNMBX-UHFFFAOYSA-N
Formula: C16H22F3NO
SMILES: CCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-435.21	kJ/mol	Joback Method
hf	-804.83	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.536		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	671.22	K	Joback Method
tc	848.42	K	Joback Method
tf	418.23	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.10	J/mol×K	671.22	Joback Method
cpg	649.46	J/mol×K	700.75	Joback Method
cpg	664.04	J/mol×K	730.29	Joback Method
cpg	677.86	J/mol×K	759.82	Joback Method
cpg	690.95	J/mol×K	789.35	Joback Method
cpg	703.33	J/mol×K	818.89	Joback Method
cpg	715.03	J/mol×K	848.42	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=U415682&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