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

Inchi: InChI=1S/C17H24F3NO/c1-3-5-7-8-12-21(11-6-4-2)17(22)13-9-10-14(18)16(20)15(13)19
InchiKey: TYBHXIWBDCVXDZ-UHFFFAOYSA-N
Formula: C17H24F3NO
SMILES: CCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 315.37

Physical Properties

Property code	Value	Unit	Source
gf	-426.79	kJ/mol	Joback Method
hf	-825.47	kJ/mol	Joback Method
hfus	46.52	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.926		Crippen Method
mcvol	243.490	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
tb	694.10	K	Joback Method
tc	871.07	K	Joback Method
tf	429.50	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.87	J/mol×K	694.10	Joback Method
cpg	704.67	J/mol×K	723.59	Joback Method
cpg	719.64	J/mol×K	753.09	Joback Method
cpg	733.84	J/mol×K	782.58	Joback Method
cpg	747.27	J/mol×K	812.08	Joback Method
cpg	759.98	J/mol×K	841.57	Joback Method
cpg	771.99	J/mol×K	871.07	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=U415684&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