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

Inchi: InChI=1S/C14H18F3NO/c1-3-5-9-18(8-4-2)14(19)10-6-7-11(15)13(17)12(10)16/h6-7H,3-
InchiKey: FEEPGZWQYCLXCT-UHFFFAOYSA-N
Formula: C14H18F3NO
SMILES: CCCCN(CCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	-452.05	kJ/mol	Joback Method
hf	-763.55	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.756		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	625.46	K	Joback Method
tc	804.34	K	Joback Method
tf	395.69	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.39	J/mol×K	625.46	Joback Method
cpg	542.80	J/mol×K	655.27	Joback Method
cpg	556.48	J/mol×K	685.09	Joback Method
cpg	569.44	J/mol×K	714.90	Joback Method
cpg	581.72	J/mol×K	744.72	Joback Method
cpg	593.34	J/mol×K	774.53	Joback Method
cpg	604.32	J/mol×K	804.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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