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

Inchi: InChI=1S/C15H20F3NO/c1-4-5-8-19(9-10(2)3)15(20)11-6-7-12(16)14(18)13(11)17/h6-7,1
InchiKey: BFPYAAYNCQNQJK-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCN(CC(C)C)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-446.07	kJ/mol	Joback Method
hf	-789.47	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.002		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	647.90	K	Joback Method
tc	828.45	K	Joback Method
tf	391.96	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.02	J/mol×K	647.90	Joback Method
cpg	596.19	J/mol×K	677.99	Joback Method
cpg	610.58	J/mol×K	708.08	Joback Method
cpg	624.19	J/mol×K	738.18	Joback Method
cpg	637.07	J/mol×K	768.27	Joback Method
cpg	649.23	J/mol×K	798.36	Joback Method
cpg	660.71	J/mol×K	828.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415679&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

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