Benzamide, 2-trifluoromethyl-N-ethyl-N-butyl-

Inchi: InChI=1S/C14H18F3NO/c1-3-5-10-18(4-2)13(19)11-8-6-7-9-12(11)14(15,16)17/h6-9H,3-
InchiKey: CMLALNHFTWYVTC-UHFFFAOYSA-N
Formula: C14H18F3NO
SMILES: CCCCN(CC)C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	-429.95	kJ/mol	Joback Method
hf	-749.36	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.968		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	612.27	K	Joback Method
tc	797.91	K	Joback Method
tf	373.07	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.85	J/mol×K	612.27	Joback Method
cpg	547.28	J/mol×K	643.21	Joback Method
cpg	561.77	J/mol×K	674.15	Joback Method
cpg	575.38	J/mol×K	705.09	Joback Method
cpg	588.14	J/mol×K	736.03	Joback Method
cpg	600.11	J/mol×K	766.97	Joback Method
cpg	611.34	J/mol×K	797.91	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=U415601&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

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