Benzamide, 4-(trifluoromethyl)-N-butyl-N-isobutyl-

Inchi: InChI=1S/C16H22F3NO/c1-4-5-10-20(11-12(2)3)15(21)13-6-8-14(9-7-13)16(17,18)19/h6

InchiKey: DZNWHQICWQNXKZ-UHFFFAOYSA-N

Formula: C16H22F3NO

SMILES: CCCCN(CC(C)C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-415.55	kJ/mol	Joback Method
hf	-795.92	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.604		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	657.59	K	Joback Method
tc	843.09	K	Joback Method
tf	380.61	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.66	J/mol×K	657.59	Joback Method
cpg	654.10	J/mol×K	688.51	Joback Method
cpg	669.55	J/mol×K	719.42	Joback Method
cpg	684.07	J/mol×K	750.34	Joback Method
cpg	697.70	J/mol×K	781.25	Joback Method
cpg	710.50	J/mol×K	812.17	Joback Method
cpg	722.53	J/mol×K	843.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415696&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