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

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

InchiKey: KIRSDKHAGVHEFJ-UHFFFAOYSA-N

Formula: C16H22F3NO

SMILES: CCCCN(CCC(C)C)C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-437.65	kJ/mol	Joback Method
hf	-810.11	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.392		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	670.78	K	Joback Method
tc	850.43	K	Joback Method
tf	403.23	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.56	J/mol×K	670.78	Joback Method
cpg	650.17	J/mol×K	700.72	Joback Method
cpg	664.97	J/mol×K	730.66	Joback Method
cpg	678.97	J/mol×K	760.61	Joback Method
cpg	692.22	J/mol×K	790.55	Joback Method
cpg	704.73	J/mol×K	820.49	Joback Method
cpg	716.53	J/mol×K	850.43	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=U415681&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