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

Inchi: InChI=1S/C12H14F3NO/c1-2-3-8-16-11(17)9-4-6-10(7-5-9)12(13,14)15/h4-7H,2-3,8H2,1
InchiKey: YSXNZUCHDLXTRZ-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CCCCNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-468.18	kJ/mol	Joback Method
hf	-722.14	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.235		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	604.24	K	Joback Method
tc	797.30	K	Joback Method
tf	370.72	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.25	J/mol×K	604.24	Joback Method
cpg	460.91	J/mol×K	636.42	Joback Method
cpg	473.69	J/mol×K	668.59	Joback Method
cpg	485.65	J/mol×K	700.77	Joback Method
cpg	496.84	J/mol×K	732.95	Joback Method
cpg	507.28	J/mol×K	765.13	Joback Method
cpg	517.04	J/mol×K	797.30	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=U407297&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