Benzamide, 4-(trifluoromethyl)-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C19H28F3NO/c1-4-6-8-9-15(3)23(14-7-5-2)18(24)16-10-12-17(13-11-16)19(20

InchiKey: FYPPAPFNRZXRHX-UHFFFAOYSA-N

Formula: C19H28F3NO

SMILES: CCCCCC(C)N(CCCC)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 343.43

Physical Properties

Property code	Value	Unit	Source
gf	-390.29	kJ/mol	Joback Method
hf	-857.84	kJ/mol	Joback Method
hfus	41.54	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.916		Crippen Method
mcvol	271.670	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	726.23	K	Joback Method
tc	909.46	K	Joback Method
tf	414.42	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.67	J/mol×K	726.23	Joback Method
cpg	821.93	J/mol×K	756.77	Joback Method
cpg	838.19	J/mol×K	787.31	Joback Method
cpg	853.49	J/mol×K	817.85	Joback Method
cpg	867.91	J/mol×K	848.38	Joback Method
cpg	881.50	J/mol×K	878.92	Joback Method
cpg	894.30	J/mol×K	909.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415700&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

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