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

Inchi: InChI=1S/C20H30F3NO/c1-3-5-7-8-9-10-11-15-24(14-6-4-2)20(25)16-12-13-17(21)19(23
InchiKey: LOZOSNOBVKKUKP-UHFFFAOYSA-N
Formula: C20H30F3NO
SMILES: CCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 357.45

Physical Properties

Property code	Value	Unit	Source
gf	-401.53	kJ/mol	Joback Method
hf	-887.39	kJ/mol	Joback Method
hfus	54.29	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.097		Crippen Method
mcvol	285.760	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	762.74	K	Joback Method
tc	942.06	K	Joback Method
tf	463.31	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.92	J/mol×K	762.74	Joback Method
cpg	876.91	J/mol×K	792.63	Joback Method
cpg	893.00	J/mol×K	822.51	Joback Method
cpg	908.21	J/mol×K	852.40	Joback Method
cpg	922.58	J/mol×K	882.29	Joback Method
cpg	936.16	J/mol×K	912.18	Joback Method
cpg	948.97	J/mol×K	942.06	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=U415686&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