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

Inchi: InChI=1S/C22H34F3NO/c1-3-5-7-8-9-10-11-12-13-17-26(16-6-4-2)22(27)18-14-15-19(23
InchiKey: WZOSPMSVAKWXLL-UHFFFAOYSA-N
Formula: C22H34F3NO
SMILES: CCCCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 385.51

Physical Properties

Property code	Value	Unit	Source
gf	-384.69	kJ/mol	Joback Method
hf	-928.67	kJ/mol	Joback Method
hfus	59.47	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	6.877		Crippen Method
mcvol	313.940	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	808.50	K	Joback Method
tc	992.49	K	Joback Method
tf	485.85	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.82	J/mol×K	808.50	Joback Method
cpg	996.65	J/mol×K	839.17	Joback Method
cpg	1013.48	J/mol×K	869.83	Joback Method
cpg	1029.38	J/mol×K	900.50	Joback Method
cpg	1044.36	J/mol×K	931.16	Joback Method
cpg	1058.49	J/mol×K	961.83	Joback Method
cpg	1071.80	J/mol×K	992.49	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=U415688&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