Benzamide, 3-trifluoromethyl-2-fluoro-N-undecyl-

Inchi: InChI=1S/C19H27F4NO/c1-2-3-4-5-6-7-8-9-10-14-24-18(25)15-12-11-13-16(17(15)20)19

InchiKey: MVULATDOJMPGSC-UHFFFAOYSA-N

Formula: C19H27F4NO

SMILES: CCCCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 361.42

Physical Properties

Property code	Value	Unit	Source
gf	-613.68	kJ/mol	Joback Method
hf	-1074.20	kJ/mol	Joback Method
hfus	49.83	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.105		Crippen Method
mcvol	273.440	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	768.65	K	Joback Method
tc	951.18	K	Joback Method
tf	462.72	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.90	J/mol×K	768.65	Joback Method
cpg	846.69	J/mol×K	799.07	Joback Method
cpg	861.59	J/mol×K	829.49	Joback Method
cpg	875.62	J/mol×K	859.92	Joback Method
cpg	888.85	J/mol×K	890.34	Joback Method
cpg	901.33	J/mol×K	920.76	Joback Method
cpg	913.09	J/mol×K	951.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407711&Units=SI

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