Benzamide, 3-trifluoromethyl-N-ethyl-N-undecyl-

Inchi: InChI=1S/C21H32F3NO/c1-3-5-6-7-8-9-10-11-12-16-25(4-2)20(26)18-14-13-15-19(17-18

InchiKey: YGHZGIWHCANJMH-UHFFFAOYSA-N

Formula: C21H32F3NO

SMILES: CCCCCCCCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 371.48

Physical Properties

Property code	Value	Unit	Source
gf	-371.01	kJ/mol	Joback Method
hf	-893.84	kJ/mol	Joback Method
hfus	50.24	kJ/mol	Joback Method
hvap	70.32	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.698		Crippen Method
mcvol	299.850	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	772.43	K	Joback Method
tc	955.16	K	Joback Method
tf	451.96	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.64	J/mol×K	772.43	Joback Method
cpg	938.27	J/mol×K	802.89	Joback Method
cpg	954.91	J/mol×K	833.34	Joback Method
cpg	970.61	J/mol×K	863.80	Joback Method
cpg	985.43	J/mol×K	894.25	Joback Method
cpg	999.42	J/mol×K	924.71	Joback Method
cpg	1012.66	J/mol×K	955.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415580&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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