Benzamide, 3-trifluoromethyl-N-ethyl-N-pentyl-

Inchi: InChI=1S/C15H20F3NO/c1-3-5-6-10-19(4-2)14(20)12-8-7-9-13(11-12)15(16,17)18/h7-9,1
InchiKey: HSGMVESYUFEISK-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-421.53	kJ/mol	Joback Method
hf	-770.00	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	56.96	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.358		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	635.15	K	Joback Method
tc	819.13	K	Joback Method
tf	384.34	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.89	J/mol×K	635.15	Joback Method
cpg	599.70	J/mol×K	665.81	Joback Method
cpg	614.57	J/mol×K	696.48	Joback Method
cpg	628.54	J/mol×K	727.14	Joback Method
cpg	641.67	J/mol×K	757.80	Joback Method
cpg	654.00	J/mol×K	788.47	Joback Method
cpg	665.58	J/mol×K	819.13	Joback Method

Sources

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=U415572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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