Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-ethyl-

Inchi: InChI=1S/C15H19F4NO/c1-3-5-6-10-20(4-2)14(21)11-8-7-9-12(13(11)16)15(17,18)19/h7

InchiKey: AGBKCCRMMAMSPZ-UHFFFAOYSA-N

Formula: C15H19F4NO

SMILES: CCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 305.31

Physical Properties

Property code	Value	Unit	Source
gf	-625.97	kJ/mol	Joback Method
hf	-977.58	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.497		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	639.40	K	Joback Method
tc	817.54	K	Joback Method
tf	397.45	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.69	J/mol×K	639.40	Joback Method
cpg	606.70	J/mol×K	669.09	Joback Method
cpg	620.85	J/mol×K	698.78	Joback Method
cpg	634.18	J/mol×K	728.47	Joback Method
cpg	646.74	J/mol×K	758.16	Joback Method
cpg	658.56	J/mol×K	787.85	Joback Method
cpg	669.69	J/mol×K	817.54	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=U415525&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