Benzamide, 3-fluoro-5-trifluoromethyl-N-nonyl-

Inchi: InChI=1S/C17H23F4NO/c1-2-3-4-5-6-7-8-9-22-16(23)13-10-14(17(19,20)21)12-15(18)11
InchiKey: JNBAUMHSUFSUIB-UHFFFAOYSA-N
Formula: C17H23F4NO
SMILES: CCCCCCCCCNC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 333.36

Physical Properties

Property code	Value	Unit	Source
gf	-630.52	kJ/mol	Joback Method
hf	-1032.92	kJ/mol	Joback Method
hfus	44.65	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.325		Crippen Method
mcvol	245.260	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	722.89	K	Joback Method
tc	904.04	K	Joback Method
tf	440.18	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.67	J/mol×K	722.89	Joback Method
cpg	732.72	J/mol×K	753.08	Joback Method
cpg	746.92	J/mol×K	783.27	Joback Method
cpg	760.29	J/mol×K	813.47	Joback Method
cpg	772.90	J/mol×K	843.66	Joback Method
cpg	784.77	J/mol×K	873.85	Joback Method
cpg	795.95	J/mol×K	904.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407859&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