Benzamide, 2-trifluoromethyl-5-fluoro-N-decyl-

Inchi: InChI=1S/C18H25F4NO/c1-2-3-4-5-6-7-8-9-12-23-17(24)15-13-14(19)10-11-16(15)18(20
InchiKey: FXJAKWJSVBTGDM-UHFFFAOYSA-N
Formula: C18H25F4NO
SMILES: CCCCCCCCCCNC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 347.39

Physical Properties

Property code	Value	Unit	Source
gf	-622.10	kJ/mol	Joback Method
hf	-1053.56	kJ/mol	Joback Method
hfus	47.24	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.715		Crippen Method
mcvol	259.350	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	745.77	K	Joback Method
tc	927.32	K	Joback Method
tf	451.45	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.78	J/mol×K	745.77	Joback Method
cpg	789.20	J/mol×K	776.03	Joback Method
cpg	803.75	J/mol×K	806.29	Joback Method
cpg	817.45	J/mol×K	836.55	Joback Method
cpg	830.37	J/mol×K	866.81	Joback Method
cpg	842.55	J/mol×K	897.06	Joback Method
cpg	854.03	J/mol×K	927.32	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=U407685&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