Benzamide, 2,3,4-trifluoro-N-nonyl-

Inchi: InChI=1S/C16H22F3NO/c1-2-3-4-5-6-7-8-11-20-16(21)12-9-10-13(17)15(19)14(12)18/h9
InchiKey: PROFNFFAEGULRF-UHFFFAOYSA-N
Formula: C16H22F3NO
SMILES: CCCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-456.60	kJ/mol	Joback Method
hf	-818.89	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.584		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	708.95	K	Joback Method
tc	890.18	K	Joback Method
tf	438.42	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.82	J/mol×K	708.95	Joback Method
cpg	666.58	J/mol×K	739.15	Joback Method
cpg	680.57	J/mol×K	769.36	Joback Method
cpg	693.80	J/mol×K	799.56	Joback Method
cpg	706.30	J/mol×K	829.77	Joback Method
cpg	718.09	J/mol×K	859.97	Joback Method
cpg	729.20	J/mol×K	890.18	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=U407268&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