Benzamide, 4-(trifluoromethyl)-N-nonyl-

Inchi: InChI=1S/C17H24F3NO/c1-2-3-4-5-6-7-8-13-21-16(22)14-9-11-15(12-10-14)17(18,19)20
InchiKey: HCGYWGWRMCDBKP-UHFFFAOYSA-N
Formula: C17H24F3NO
SMILES: CCCCCCCCCNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 315.37

Physical Properties

Property code	Value	Unit	Source
gf	-426.08	kJ/mol	Joback Method
hf	-825.34	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.186		Crippen Method
mcvol	243.490	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	718.64	K	Joback Method
tc	904.16	K	Joback Method
tf	427.07	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.38	J/mol×K	718.64	Joback Method
cpg	726.05	J/mol×K	749.56	Joback Method
cpg	740.81	J/mol×K	780.48	Joback Method
cpg	754.69	J/mol×K	811.40	Joback Method
cpg	767.75	J/mol×K	842.32	Joback Method
cpg	780.03	J/mol×K	873.24	Joback Method
cpg	791.60	J/mol×K	904.16	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=U407305&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