

Benzamide, 3-trifluoromethyl-2-fluoro-N-nonyl-

Inchi:	InChI=1S/C17H23F4NO/c1-2-3-4-5-6-7-8-12-22-16(23)13-10-9-11-14(15(13)18)17(19,20
InchiKey:	OYOZLQRVKUMGNZ-UHFFFAOYSA-N
Formula:	C17H23F4NO
SMILES:	CCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1F
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
rinpola	2028.00		NIST Webbook
rinpola	2028.00		NIST Webbook
tb	722.89	K	Joback Method
tc	904.04	K	Joback Method
tf	440.18	K	Joback Method
vc	0.982	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U407709&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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