Benzamide, 2,5-di(trifluoromethyl)-N-nonyl-

Inchi: InChI=1S/C18H23F6NO/c1-2-3-4-5-6-7-8-11-25-16(26)14-12-13(17(19,20)21)9-10-15(14
InchiKey: IVVMNRGVPOYQKI-UHFFFAOYSA-N
Formula: C18H23F6NO
SMILES: CCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 383.37

Physical Properties

Property code	Value	Unit	Source
gf	-1008.88	kJ/mol	Joback Method
hf	-1454.53	kJ/mol	Joback Method
hfus	45.99	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.205		Crippen Method
mcvol	262.890	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	1947.00		NIST Webbook
tb	741.08	K	Joback Method
tc	919.04	K	Joback Method
tf	455.05	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.19	J/mol×K	741.08	Joback Method
cpg	805.93	J/mol×K	770.74	Joback Method
cpg	819.81	J/mol×K	800.40	Joback Method
cpg	832.86	J/mol×K	830.06	Joback Method
cpg	845.15	J/mol×K	859.72	Joback Method
cpg	856.73	J/mol×K	889.38	Joback Method
cpg	867.66	J/mol×K	919.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407926&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume