Benzamide, N,N-dinonyl-3-trifluoromethyl-

Inchi: InChI=1S/C26H42F3NO/c1-3-5-7-9-11-13-15-20-30(21-16-14-12-10-8-6-4-2)25(31)23-18
InchiKey: QQCGQHFIKQFMFM-UHFFFAOYSA-N
Formula: C26H42F3NO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 441.61

Physical Properties

Property code	Value	Unit	Source
gf	-328.91	kJ/mol	Joback Method
hf	-997.04	kJ/mol	Joback Method
hfus	63.19	kJ/mol	Joback Method
hvap	81.45	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	8.649		Crippen Method
mcvol	370.300	ml/mol	McGowan Method
pc	838.70	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	886.83	K	Joback Method
tc	1085.75	K	Joback Method
tf	508.31	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.17	J/mol×K	886.83	Joback Method
cpg	1245.87	J/mol×K	919.98	Joback Method
cpg	1264.42	J/mol×K	953.14	Joback Method
cpg	1281.91	J/mol×K	986.29	Joback Method
cpg	1298.44	J/mol×K	1019.45	Joback Method
cpg	1314.09	J/mol×K	1052.60	Joback Method
cpg	1328.96	J/mol×K	1085.75	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=U308231&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