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

Inchi: InChI=1S/C20H27F6NO/c1-2-3-4-5-6-7-8-9-10-13-27-18(28)16-14-15(19(21,22)23)11-12
InchiKey: TYHSQPFKJGSRAC-UHFFFAOYSA-N
Formula: C20H27F6NO
SMILES: CCCCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 411.42

Physical Properties

Property code	Value	Unit	Source
gf	-992.04	kJ/mol	Joback Method
hf	-1495.81	kJ/mol	Joback Method
hfus	51.17	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.985		Crippen Method
mcvol	291.070	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	2140.00		NIST Webbook
tb	786.84	K	Joback Method
tc	968.23	K	Joback Method
tf	477.59	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.49	J/mol×K	786.84	Joback Method
cpg	921.01	J/mol×K	817.07	Joback Method
cpg	935.63	J/mol×K	847.30	Joback Method
cpg	949.40	J/mol×K	877.53	Joback Method
cpg	962.39	J/mol×K	907.77	Joback Method
cpg	974.65	J/mol×K	938.00	Joback Method
cpg	986.25	J/mol×K	968.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407928&Units=SI
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

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