

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

Inchi:	InChI=1S/C14H15F6NO/c1-2-3-4-7-21-12(22)10-8-9(13(15,16)17)5-6-11(10)14(18,19)20
InchiKey:	XFEQGKNTHDYBKO-UHFFFAOYSA-N
Formula:	C14H15F6NO
SMILES:	CCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	327.27

Physical Properties

Property code	Value	Unit	Source
gf	-1042.56	kJ/mol	Joback Method
hf	-1371.97	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.644		Crippen Method
mvol	206.530	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
tb	649.56	K	Joback Method
tc	827.26	K	Joback Method
tf	409.97	K	Joback Method
vc	0.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.13	J/mol×K	649.56	Joback Method
cpg	588.35	J/mol×K	679.18	Joback Method
cpg	600.74	J/mol×K	708.79	Joback Method
cpg	612.34	J/mol×K	738.41	Joback Method
cpg	623.20	J/mol×K	768.03	Joback Method
cpg	633.37	J/mol×K	797.64	Joback Method
cpg	642.91	J/mol×K	827.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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