Benzamide, N-(3-methylphenyl)-2,3,4,5,6-pentafluoro-

Inchi: InChI=1S/C14H8F5NO/c1-6-3-2-4-7(5-6)20-14(21)8-9(15)11(17)13(19)12(18)10(8)16/h2-

InchiKey: MYHFRQGGHKYKJB-UHFFFAOYSA-N

Formula: C14H8F5NO

SMILES: Cc1cccc(NC(=O)c2c(F)c(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 301.21

Physical Properties

Property code	Value	Unit	Source
gf	-779.54	kJ/mol	Joback Method
hf	-967.71	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	3.943		Crippen Method
mcvol	181.000	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	703.35	K	Joback Method
tc	904.60	K	Joback Method
tf	481.04	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.06	J/mol×K	703.35	Joback Method
cpg	485.01	J/mol×K	736.89	Joback Method
cpg	495.24	J/mol×K	770.43	Joback Method
cpg	504.78	J/mol×K	803.98	Joback Method
cpg	513.63	J/mol×K	837.52	Joback Method
cpg	521.83	J/mol×K	871.06	Joback Method
cpg	529.39	J/mol×K	904.60	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=U307376&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