Propanamide, N-(3-methylphenyl)-2,2,3,3,3-pentafluoro-

Inchi: InChI=1S/C10H8F5NO/c1-6-3-2-4-7(5-6)16-8(17)9(11,12)10(13,14)15/h2-5H,1H3,(H,16,1

InchiKey: UMEFLILOWZCUAN-UHFFFAOYSA-N

Formula: C10H8F5NO

SMILES: Cc1cccc(NC(=O)C(F)(F)C(F)(F)F)c1

Mol. weight [g/mol]: 253.17

Physical Properties

Property code	Value	Unit	Source
gf	-871.80	kJ/mol	Joback Method
hf	-1081.83	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	47.30	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.131		Crippen Method
mcvol	148.400	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1179.00		NIST Webbook
tb	553.79	K	Joback Method
tc	744.76	K	Joback Method
tf	351.78	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.72	J/mol×K	553.79	Joback Method
cpg	383.74	J/mol×K	585.62	Joback Method
cpg	394.86	J/mol×K	617.45	Joback Method
cpg	405.13	J/mol×K	649.27	Joback Method
cpg	414.61	J/mol×K	681.10	Joback Method
cpg	423.35	J/mol×K	712.93	Joback Method
cpg	431.40	J/mol×K	744.76	Joback Method

Sources

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=U307330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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