Propanamide, N-(4-methoxyphenyl)-2,2,3,3,3-pentafluoro-

Inchi: InChI=1S/C10H8F5NO2/c1-18-7-4-2-6(3-5-7)16-8(17)9(11,12)10(13,14)15/h2-5H,1H3,(H

InchiKey: UADJWOUXOILVLP-UHFFFAOYSA-N

Formula: C10H8F5NO2

SMILES: COc1ccc(NC(=O)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 269.17

Physical Properties

Property code	Value	Unit	Source
gf	-976.80	kJ/mol	Joback Method
hf	-1214.05	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.831		Crippen Method
mcvol	154.270	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1355.00		NIST Webbook
tb	576.21	K	Joback Method
tc	765.84	K	Joback Method
tf	374.01	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.74	J/mol×K	576.21	Joback Method
cpg	407.37	J/mol×K	607.81	Joback Method
cpg	418.18	J/mol×K	639.42	Joback Method
cpg	428.20	J/mol×K	671.02	Joback Method
cpg	437.48	J/mol×K	702.63	Joback Method
cpg	446.06	J/mol×K	734.23	Joback Method
cpg	453.98	J/mol×K	765.84	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=U307332&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