Butanamide, N-(4-methoxyphenyl)-2,2,3,3,4,4,4-heptafluoro-

Inchi: InChI=1S/C11H8F7NO2/c1-21-7-4-2-6(3-5-7)19-8(20)9(12,13)10(14,15)11(16,17)18/h2-5

InchiKey: DQKFVVPVNVSDOM-UHFFFAOYSA-N

Formula: C11H8F7NO2

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

Mol. weight [g/mol]: 319.18

Physical Properties

Property code	Value	Unit	Source
gf	-1355.16	kJ/mol	Joback Method
hf	-1635.66	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	49.00	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.467		Crippen Method
mcvol	171.900	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	594.40	K	Joback Method
tc	775.75	K	Joback Method
tf	388.88	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.05	J/mol×K	594.40	Joback Method
cpg	474.78	J/mol×K	624.62	Joback Method
cpg	485.63	J/mol×K	654.85	Joback Method
cpg	495.64	J/mol×K	685.07	Joback Method
cpg	504.87	J/mol×K	715.30	Joback Method
cpg	513.38	J/mol×K	745.52	Joback Method
cpg	521.21	J/mol×K	775.75	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=U307278&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