Methyl 2-(N-heptafluorobutyrylamino)benzoate

Inchi: InChI=1S/C12H8F7NO3/c1-23-8(21)6-4-2-3-5-7(6)20-9(22)10(13,14)11(15,16)12(17,18)1
InchiKey: OSASKXXYHKHJKT-UHFFFAOYSA-N
Formula: C12H8F7NO3
SMILES: COC(=O)c1ccccc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 347.19

Physical Properties

Property code	Value	Unit	Source
gf	-1475.66	kJ/mol	Joback Method
hf	-1768.88	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	57.97	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.245		Crippen Method
mcvol	187.560	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	671.15	K	Joback Method
tc	858.39	K	Joback Method
tf	450.08	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.33	J/mol×K	671.15	Joback Method
cpg	537.90	J/mol×K	702.36	Joback Method
cpg	547.61	J/mol×K	733.56	Joback Method
cpg	556.53	J/mol×K	764.77	Joback Method
cpg	564.71	J/mol×K	795.97	Joback Method
cpg	572.21	J/mol×K	827.18	Joback Method
cpg	579.10	J/mol×K	858.39	Joback Method

Sources

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=U374366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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