MTMC, TFA

Inchi: InChI=1S/C11H10F3NO3/c1-7-4-3-5-8(6-7)18-10(17)15(2)9(16)11(12,13)14/h3-6H,1-2H3
InchiKey: HHPDTFUGBDDVIV-UHFFFAOYSA-N
Formula: C11H10F3NO3
SMILES: Cc1cccc(OC(=O)N(C)C(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 261.20

Physical Properties

Property code	Value	Unit	Source
gf	-689.13	kJ/mol	Joback Method
hf	-932.24	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.515		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	619.92	K	Joback Method
tc	818.20	K	Joback Method
tf	411.42	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.97	J/mol×K	619.92	Joback Method
cpg	439.06	J/mol×K	652.97	Joback Method
cpg	450.31	J/mol×K	686.01	Joback Method
cpg	460.75	J/mol×K	719.06	Joback Method
cpg	470.44	J/mol×K	752.11	Joback Method
cpg	479.39	J/mol×K	785.16	Joback Method

cpg	487.66	J/mol×K	818.20	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=R522155&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