carbaryl, TFA

Inchi: InChI=1S/C14H10F3NO3/c1-18(12(19)14(15,16)17)13(20)21-11-8-4-6-9-5-2-3-7-10(9)11
InchiKey: NDKMVMNLDKNHGZ-UHFFFAOYSA-N
Formula: C14H10F3NO3
SMILES: CN(C(=O)Oc1cccc2ccccc12)C(=O)C(F)(F)F
Mol. weight [g/mol]: 297.23

Physical Properties

Property code	Value	Unit	Source
gf	-557.22	kJ/mol	Joback Method
hf	-803.09	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.359		Crippen Method
mcvol	189.200	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	707.54	K	Joback Method
tc	919.95	K	Joback Method
tf	477.93	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.28	J/mol×K	707.54	Joback Method
cpg	524.98	J/mol×K	742.94	Joback Method
cpg	535.75	J/mol×K	778.34	Joback Method
cpg	545.64	J/mol×K	813.74	Joback Method
cpg	554.75	J/mol×K	849.15	Joback Method
cpg	563.14	J/mol×K	884.55	Joback Method

cpg	570.90	J/mol×K	919.95	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=R522100&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