Dihydrocapsaicin, O-trifluoroacetyl-

Inchi: InChI=1S/C20H28F3NO4/c1-14(2)8-6-4-5-7-9-18(25)24-13-15-10-11-16(17(12-15)27-3)2
InchiKey: RXVYELDAQCJVFS-UHFFFAOYSA-N
Formula: C20H28F3NO4
SMILES: COc1cc(CNC(=O)CCCCCCC(C)C)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 403.44

Physical Properties

Property code	Value	Unit	Source
gf	-751.81	kJ/mol	Joback Method
hf	-1281.03	kJ/mol	Joback Method
hfus	49.79	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.776		Crippen Method
mcvol	299.070	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2193.30		NIST Webbook
rinpol	2193.30		NIST Webbook
tb	890.53	K	Joback Method
tc	1092.96	K	Joback Method
tf	552.79	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.02	J/mol×K	890.53	Joback Method
cpg	973.41	J/mol×K	924.27	Joback Method
cpg	986.68	J/mol×K	958.01	Joback Method
cpg	998.87	J/mol×K	991.74	Joback Method
cpg	1010.01	J/mol×K	1025.48	Joback Method
cpg	1020.15	J/mol×K	1059.22	Joback Method
cpg	1029.32	J/mol×K	1092.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353108&Units=SI
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

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

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