Dihydrocapsaicin, O-pentafluoropropionyl-

Inchi: InChI=1S/C21H28F5NO4/c1-14(2)8-6-4-5-7-9-18(28)27-13-15-10-11-16(17(12-15)30-3)3
InchiKey: DJARFYKDJKEUKK-UHFFFAOYSA-N
Formula: C21H28F5NO4
SMILES: COc1cc(CNC(=O)CCCCCCC(C)C)ccc1OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 453.44

Physical Properties

Property code	Value	Unit	Source
gf	-1130.17	kJ/mol	Joback Method
hf	-1702.64	kJ/mol	Joback Method
hfus	51.13	kJ/mol	Joback Method
hvap	83.62	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.411		Crippen Method
mcvol	316.700	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2186.50		NIST Webbook
rinpol	2186.50		NIST Webbook
tb	908.72	K	Joback Method
tc	1112.88	K	Joback Method
tf	567.66	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.22	J/mol×K	908.72	Joback Method
cpg	1047.43	J/mol×K	942.75	Joback Method
cpg	1060.54	J/mol×K	976.77	Joback Method
cpg	1072.61	J/mol×K	1010.80	Joback Method
cpg	1083.71	J/mol×K	1044.82	Joback Method
cpg	1093.91	J/mol×K	1078.85	Joback Method
cpg	1103.25	J/mol×K	1112.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353106&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

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