Dihydrocapsaicin, O-heptafluorobutyryl-

Inchi: InChI=1S/C22H28F7NO4/c1-14(2)8-6-4-5-7-9-18(31)30-13-15-10-11-16(17(12-15)33-3)3
InchiKey: XMFLKZAAVZSFNM-UHFFFAOYSA-N
Formula: C22H28F7NO4
SMILES: COc1cc(CNC(=O)CCCCCCC(C)C)ccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 503.45

Physical Properties

Property code	Value	Unit	Source
gf	-1508.53	kJ/mol	Joback Method
hf	-2124.25	kJ/mol	Joback Method
hfus	52.47	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.046		Crippen Method
mcvol	334.330	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	2220.00		NIST Webbook
tb	926.91	K	Joback Method
tc	1135.03	K	Joback Method
tf	582.53	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.43	J/mol×K	926.91	Joback Method
cpg	1121.62	J/mol×K	961.60	Joback Method
cpg	1134.74	J/mol×K	996.28	Joback Method
cpg	1146.89	J/mol×K	1030.97	Joback Method
cpg	1158.14	J/mol×K	1065.66	Joback Method
cpg	1168.61	J/mol×K	1100.34	Joback Method
cpg	1178.37	J/mol×K	1135.03	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=U353104&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