Dihydrocapsaicin, O-acetyl-

Inchi: InChI=1S/C20H31NO4/c1-15(2)9-7-5-6-8-10-20(23)21-14-17-11-12-18(25-16(3)22)19(13
InchiKey: FABOGEJIOHNBJZ-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: COc1cc(CNC(=O)CCCCCCC(C)C)ccc1OC(C)=O
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
gf	-170.22	kJ/mol	Joback Method
hf	-683.95	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	88.07	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.233		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	2736.50		NIST Webbook
rinpol	2736.50		NIST Webbook
tb	895.95	K	Joback Method
tc	1103.67	K	Joback Method
tf	548.60	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.81	J/mol×K	895.95	Joback Method
cpg	952.08	J/mol×K	930.57	Joback Method
cpg	966.12	J/mol×K	965.19	Joback Method
cpg	978.94	J/mol×K	999.81	Joback Method
cpg	990.56	J/mol×K	1034.43	Joback Method
cpg	1001.01	J/mol×K	1069.05	Joback Method
cpg	1010.30	J/mol×K	1103.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353103&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

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