Dihydrocapsaicin, N-methyl-, methyl ether

Inchi: InChI=1S/C20H33NO3/c1-16(2)10-8-6-7-9-11-20(22)21(3)15-17-12-13-18(23-4)19(14-17
InchiKey: JJWOOWFCJRLRJG-UHFFFAOYSA-N
Formula: C20H33NO3
SMILES: COc1ccc(CN(C)C(=O)CCCCCCC(C)C)cc1OC
Mol. weight [g/mol]: 335.48

Physical Properties

Property code	Value	Unit	Source
gf	-19.91	kJ/mol	Joback Method
hf	-557.31	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	76.94	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.659		Crippen Method
mcvol	292.190	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2619.30		NIST Webbook
rinpol	2619.30		NIST Webbook
tb	804.35	K	Joback Method
tc	998.83	K	Joback Method
tf	478.48	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.52	J/mol×K	804.35	Joback Method
cpg	917.43	J/mol×K	836.76	Joback Method
cpg	934.23	J/mol×K	869.18	Joback Method
cpg	949.93	J/mol×K	901.59	Joback Method
cpg	964.55	J/mol×K	934.00	Joback Method
cpg	978.13	J/mol×K	966.42	Joback Method
cpg	990.69	J/mol×K	998.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353102&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