cis-3-Nonen-1-ol, pentafluoropropionate

Inchi: InChI=1S/C12H17F5O2/c1-2-3-4-5-6-7-8-9-19-10(18)11(13,14)12(15,16)17/h6-7H,2-5,8-
InchiKey: VXZOOHSAUUTTGX-SREVYHEPSA-N
Formula: C12H17F5O2
SMILES: CCCCCC=CCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 288.25

Physical Properties

Property code	Value	Unit	Source
gf	-1071.91	kJ/mol	Joback Method
hf	-1416.64	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.254		Crippen Method
mcvol	191.930	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	1164.50		NIST Webbook
tb	544.30	K	Joback Method
tc	702.71	K	Joback Method
tf	299.87	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.49	J/mol×K	544.30	Joback Method
cpg	506.38	J/mol×K	570.70	Joback Method
cpg	519.55	J/mol×K	597.10	Joback Method
cpg	532.03	J/mol×K	623.50	Joback Method
cpg	543.85	J/mol×K	649.90	Joback Method
cpg	555.04	J/mol×K	676.31	Joback Method
cpg	565.64	J/mol×K	702.71	Joback Method

Sources

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=U352766&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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