cis-3-Nonen-1-ol, trifluoroacetate

Inchi: InChI=1S/C11H17F3O2/c1-2-3-4-5-6-7-8-9-16-10(15)11(12,13)14/h6-7H,2-5,8-9H2,1H3/
InchiKey: LYTSCVXMFNQMSH-SREVYHEPSA-N
Formula: C11H17F3O2
SMILES: CCCCCC=CCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 238.25

Physical Properties

Property code	Value	Unit	Source
gf	-693.55	kJ/mol	Joback Method
hf	-995.03	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.619		Crippen Method
mcvol	174.300	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1147.90		NIST Webbook
rinpol	1146.30		NIST Webbook
rinpol	1146.30		NIST Webbook
tb	526.11	K	Joback Method
tc	690.56	K	Joback Method
tf	285.00	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.95	J/mol×K	526.11	Joback Method
cpg	438.58	J/mol×K	553.52	Joback Method
cpg	451.56	J/mol×K	580.93	Joback Method
cpg	463.92	J/mol×K	608.33	Joback Method
cpg	475.68	J/mol×K	635.74	Joback Method
cpg	486.86	J/mol×K	663.15	Joback Method
cpg	497.49	J/mol×K	690.56	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=U352771&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