Nonadecyl trifluoroacetate

Other names: Nonadecyl 2,2,2-trifluoroacetate
1-Nonadecanol, trifluoroacetate
Inchi: InChI=1S/C21H39F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-26-20(25)21
InchiKey: WEKMLKHOURBVLB-UHFFFAOYSA-N
Formula: C21H39F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 380.53

Physical Properties

Property code	Value	Unit	Source
gf	-689.57	kJ/mol	Joback Method
hf	-1318.65	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.744		Crippen Method
mcvol	319.500	ml/mol	McGowan Method
pc	916.05	kPa	Joback Method
rinpol	2100.40		NIST Webbook
rinpol	2100.40		NIST Webbook
tb	750.75	K	Joback Method
tc	920.39	K	Joback Method
tf	402.78	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.22	J/mol×K	750.75	Joback Method
cpg	1012.46	J/mol×K	779.02	Joback Method
cpg	1030.75	J/mol×K	807.30	Joback Method
cpg	1048.13	J/mol×K	835.57	Joback Method
cpg	1064.63	J/mol×K	863.84	Joback Method
cpg	1080.29	J/mol×K	892.11	Joback Method

cpg	1095.14	J/mol×K	920.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351763&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