Nonadecyl pentafluoropropionate

Other names: Nonadecyl 2,2,3,3,3-pentafluoropropanoate
1-Nonadecanol, pentafluoropropionate
Inchi: InChI=1S/C22H39F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-29-20(28)21
InchiKey: XNZQXRPFPKNTIG-UHFFFAOYSA-N
Formula: C22H39F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 430.54

Physical Properties

Property code	Value	Unit	Source
gf	-1067.93	kJ/mol	Joback Method
hf	-1740.26	kJ/mol	Joback Method
hfus	56.09	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	8.379		Crippen Method
mcvol	337.130	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	2099.60		NIST Webbook
tb	768.94	K	Joback Method
tc	941.42	K	Joback Method
tf	417.65	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.49	J/mol×K	768.94	Joback Method
cpg	1089.81	J/mol×K	797.69	Joback Method
cpg	1108.12	J/mol×K	826.43	Joback Method
cpg	1125.47	J/mol×K	855.18	Joback Method
cpg	1141.92	J/mol×K	883.93	Joback Method
cpg	1157.51	J/mol×K	912.67	Joback Method
cpg	1172.29	J/mol×K	941.42	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=U351888&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