Nonadecyl heptafluorobutyrate

Other names:	Nonadecyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Nonadecanol, heptafluorobutyrate
	Nonadecyl perfluorobutyrate
Inchi:	InChI=1S/C23H39F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-32-20(31)21
InchiKey:	NJWZHUGJBXGPMH-UHFFFAOYSA-N
Formula:	C23H39F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	480.54

Physical Properties

Property code	Value	Unit	Source
gf	-1446.29	kJ/mol	Joback Method
hf	-2161.87	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-9.60		Crippen Method
logp	9.014		Crippen Method
mcvol	354.760	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	2126.50		NIST Webbook
rinpol	2126.50		NIST Webbook
tb	787.13	K	Joback Method
tc	964.37	K	Joback Method
tf	432.52	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.87	J/mol×K	787.13	Joback Method
cpg	1167.41	J/mol×K	816.67	Joback Method
cpg	1185.88	J/mol×K	846.21	Joback Method
cpg	1203.33	J/mol×K	875.75	Joback Method
cpg	1219.86	J/mol×K	905.29	Joback Method

cpg	1235.51	J/mol×K	934.83	Joback Method
cpg	1250.37	J/mol×K	964.37	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=U351839&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