

Nonyl 2,3,4,5,6-pentafluorobenzoate

Other names:	nonyl pentafluorobenzoate
Inchi:	InChI=1S/C16H19F5O2/c1-2-3-4-5-6-7-8-9-23-16(22)10-11(17)13(19)15(21)14(20)12(10)
InchiKey:	JYFVJMHUQOOXPH-UHFFFAOYSA-N
Formula:	C16H19F5O2
SMILES:	CCCCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	338.31

Physical Properties

Property code	Value	Unit	Source
gf	-1059.87	kJ/mol	Joback Method
hf	-1419.74	kJ/mol	Joback Method
hfus	47.48	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.290		Crippen Method
mcvol	228.830	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1713.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	2002.00		NIST Webbook
tb	689.70	K	Joback Method
tc	859.82	K	Joback Method
tf	434.21	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.55	J/mol×K	689.70	Joback Method
cpg	651.29	J/mol×K	718.05	Joback Method
cpg	664.38	J/mol×K	746.41	Joback Method
cpg	676.84	J/mol×K	774.76	Joback Method
cpg	688.67	J/mol×K	803.12	Joback Method
cpg	699.87	J/mol×K	831.47	Joback Method
cpg	710.46	J/mol×K	859.82	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=U373593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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