

heptafluorobutanoic acid, nonyl ester

Other names:	Nonyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Nonanol, heptafluorobutyrate Nonyl perfluorobutyrate Nonyl heptafluorobutanoate
Inchi:	InChI=1S/C13H19F7O2/c1-2-3-4-5-6-7-8-9-22-10(21)11(14,15)12(16,17)13(18,19)20/h2-
InchiKey:	KKMYDVWFFLRAAN-UHFFFAOYSA-N
Formula:	C13H19F7O2
SMILES:	CCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	340.28

Physical Properties

Property code	Value	Unit	Source
hf	-2031.90	kJ/mol	Cheméo Relay (1.0)
hfus	31.53	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.04		Cheméo Relay (1.0)
logp	5.113		Crippen Method
mcvol	213.860	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1201.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1208.90		NIST Webbook
rinpol	1208.90		NIST Webbook
rinpol	1201.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	468.31	K	Cheméo Relay (1.0)
tc	584.20	K	Cheméo Relay (1.0)
tf	227.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	579.90	J/mol×K	558.33	Joback Method
cpg	594.35	J/mol×K	583.11	Joback Method
cpg	608.07	J/mol×K	607.89	Joback Method
cpg	621.08	J/mol×K	632.67	Joback Method
cpg	633.42	J/mol×K	657.45	Joback Method
cpg	645.12	J/mol×K	682.22	Joback Method
cpg	656.20	J/mol×K	707.00	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C959297304&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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

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