Fumaric acid, nonyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H24F8O4/c1-2-3-4-5-6-7-8-11-29-13(27)9-10-14(28)30-12-16(21,22)18(25

InchiKey: NFNZTVNFRUMRQD-MDZDMXLPSA-N

Formula: C18H24F8O4

SMILES: CCCCCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.37

Physical Properties

Property code	Value	Unit	Source
gf	-1839.34	kJ/mol	Joback Method
hf	-2387.64	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.551		Crippen Method
mcvol	289.220	ml/mol	McGowan Method
pc	1042.60	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
tb	752.01	K	Joback Method
tc	922.27	K	Joback Method
tf	428.84	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.90	J/mol×K	752.01	Joback Method
cpg	906.45	J/mol×K	780.39	Joback Method
cpg	920.13	J/mol×K	808.76	Joback Method
cpg	933.01	J/mol×K	837.14	Joback Method
cpg	945.13	J/mol×K	865.52	Joback Method
cpg	956.55	J/mol×K	893.89	Joback Method
cpg	967.32	J/mol×K	922.27	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=U348785&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