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

Inchi: InChI=1S/C21H32F8O4/c1-4-7-8-9-10-11-12-13-32-16(30)18(5-2,6-3)17(31)33-14-19(24

InchiKey: PJRBAMSXPWRUEJ-UHFFFAOYSA-N

Formula: C21H32F8O4

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

Mol. weight [g/mol]: 500.46

Physical Properties

Property code	Value	Unit	Source
gf	-1891.46	kJ/mol	Joback Method
hf	-2575.53	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.801		Crippen Method
mcvol	335.790	ml/mol	McGowan Method
pc	855.96	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	813.26	K	Joback Method
tc	995.76	K	Joback Method
tf	470.15	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.30	J/mol×K	813.26	Joback Method
cpg	1109.94	J/mol×K	843.68	Joback Method
cpg	1125.55	J/mol×K	874.09	Joback Method
cpg	1140.19	J/mol×K	904.51	Joback Method
cpg	1153.95	J/mol×K	934.93	Joback Method
cpg	1166.89	J/mol×K	965.35	Joback Method
cpg	1179.10	J/mol×K	995.76	Joback Method

Sources

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=U370657&Units=SI
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
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