Diethylmalonic acid, nonyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C19H31F5O4/c1-4-7-8-9-10-11-12-13-27-15(25)17(5-2,6-3)16(26)28-14-18(20

InchiKey: VGPGODMISANVFI-UHFFFAOYSA-N

Formula: C19H31F5O4

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

Mol. weight [g/mol]: 418.44

Physical Properties

Property code	Value	Unit	Source
gf	-1324.27	kJ/mol	Joback Method
hf	-1931.89	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.827		Crippen Method
mcvol	302.300	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	773.36	K	Joback Method
tc	949.39	K	Joback Method
tf	458.42	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.67	J/mol×K	773.36	Joback Method
cpg	966.96	J/mol×K	802.70	Joback Method
cpg	982.30	J/mol×K	832.04	Joback Method
cpg	996.74	J/mol×K	861.37	Joback Method
cpg	1010.33	J/mol×K	890.71	Joback Method
cpg	1023.13	J/mol×K	920.05	Joback Method
cpg	1035.18	J/mol×K	949.39	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=U370846&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

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