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

Inchi: InChI=1S/C17H24F8O4/c1-4-7-8-9-28-12(26)14(5-2,6-3)13(27)29-10-15(20,21)17(24,25)

InchiKey: HCFZNWQEADMTNK-UHFFFAOYSA-N

Formula: C17H24F8O4

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

Mol. weight [g/mol]: 444.36

Physical Properties

Property code	Value	Unit	Source
gf	-1925.14	kJ/mol	Joback Method
hf	-2492.97	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.240		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1575.00		NIST Webbook
tb	721.74	K	Joback Method
tc	888.39	K	Joback Method
tf	425.07	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.06	J/mol×K	721.74	Joback Method
cpg	875.75	J/mol×K	749.52	Joback Method
cpg	889.56	J/mol×K	777.29	Joback Method
cpg	902.54	J/mol×K	805.07	Joback Method
cpg	914.73	J/mol×K	832.84	Joback Method
cpg	926.18	J/mol×K	860.62	Joback Method
cpg	936.96	J/mol×K	888.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U370653&Units=SI

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