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

Inchi: InChI=1S/C22H34F8O4/c1-4-7-8-9-10-11-12-13-14-33-17(31)19(5-2,6-3)18(32)34-15-20

InchiKey: QTNRKYAEISPAHE-UHFFFAOYSA-N

Formula: C22H34F8O4

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

Mol. weight [g/mol]: 514.49

Physical Properties

Property code	Value	Unit	Source
gf	-1883.04	kJ/mol	Joback Method
hf	-2596.17	kJ/mol	Joback Method
hfus	49.77	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.191		Crippen Method
mcvol	349.880	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	836.14	K	Joback Method
tc	1024.67	K	Joback Method
tf	481.42	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.36	J/mol×K	836.14	Joback Method
cpg	1170.61	J/mol×K	867.56	Joback Method
cpg	1186.77	J/mol×K	898.98	Joback Method
cpg	1201.93	J/mol×K	930.40	Joback Method
cpg	1216.16	J/mol×K	961.83	Joback Method
cpg	1229.56	J/mol×K	993.25	Joback Method
cpg	1242.21	J/mol×K	1024.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370658&Units=SI
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

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