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

Inchi: InChI=1S/C23H36F8O4/c1-4-7-8-9-10-11-12-13-14-15-34-18(32)20(5-2,6-3)19(33)35-16
InchiKey: JYAWMCDGWLDNFK-UHFFFAOYSA-N
Formula: C23H36F8O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 528.52

Physical Properties

Property code	Value	Unit	Source
gf	-1874.62	kJ/mol	Joback Method
hf	-2616.81	kJ/mol	Joback Method
hfus	52.36	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.581		Crippen Method
mcvol	363.970	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	859.02	K	Joback Method
tc	1054.55	K	Joback Method
tf	492.69	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1214.13	J/mol×K	859.02	Joback Method
cpg	1232.05	J/mol×K	891.61	Joback Method
cpg	1248.83	J/mol×K	924.20	Joback Method
cpg	1264.54	J/mol×K	956.78	Joback Method
cpg	1279.31	J/mol×K	989.37	Joback Method
cpg	1293.21	J/mol×K	1021.96	Joback Method
cpg	1306.35	J/mol×K	1054.55	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=U370659&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