Diethylmalonic acid, 2,2,3,3,4,4,4-heptafluorobutyl undecyl ester

Inchi: InChI=1S/C22H35F7O4/c1-4-7-8-9-10-11-12-13-14-15-32-17(30)19(5-2,6-3)18(31)33-16

InchiKey: DLGBJOVABFAHOP-UHFFFAOYSA-N

Formula: C22H35F7O4

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

Mol. weight [g/mol]: 496.50

Physical Properties

Property code	Value	Unit	Source
gf	-1685.79	kJ/mol	Joback Method
hf	-2394.78	kJ/mol	Joback Method
hfus	50.21	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.243		Crippen Method
mcvol	348.110	ml/mol	McGowan Method
pc	827.16	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	837.31	K	Joback Method
tc	1025.58	K	Joback Method
tf	495.83	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.55	J/mol×K	837.31	Joback Method
cpg	1162.87	J/mol×K	868.69	Joback Method
cpg	1179.13	J/mol×K	900.07	Joback Method
cpg	1194.40	J/mol×K	931.45	Joback Method
cpg	1208.77	J/mol×K	962.83	Joback Method
cpg	1222.31	J/mol×K	994.21	Joback Method
cpg	1235.12	J/mol×K	1025.58	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=U368436&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