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

Inchi: InChI=1S/C24H38F8O4/c1-4-7-8-9-10-11-12-13-14-15-16-35-19(33)21(5-2,6-3)20(34)36
InchiKey: ONKMLEDLJGXDMA-UHFFFAOYSA-N
Formula: C24H38F8O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 542.54

Physical Properties

Property code	Value	Unit	Source
gf	-1866.20	kJ/mol	Joback Method
hf	-2637.45	kJ/mol	Joback Method
hfus	54.95	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.971		Crippen Method
mcvol	378.060	ml/mol	McGowan Method
pc	728.10	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	881.90	K	Joback Method
tc	1085.48	K	Joback Method
tf	503.96	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.56	J/mol×K	881.90	Joback Method
cpg	1294.23	J/mol×K	915.83	Joback Method
cpg	1311.68	J/mol×K	949.76	Joback Method
cpg	1328.03	J/mol×K	983.69	Joback Method
cpg	1343.38	J/mol×K	1017.62	Joback Method
cpg	1357.85	J/mol×K	1051.55	Joback Method
cpg	1371.55	J/mol×K	1085.48	Joback Method

Sources

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=U370660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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