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

Inchi: InChI=1S/C27H45F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-37-22(35)24(5-2,
InchiKey: MBRJCEPIVGMNMG-UHFFFAOYSA-N
Formula: C27H45F7O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 566.63

Physical Properties

Property code	Value	Unit	Source
gf	-1643.69	kJ/mol	Joback Method
hf	-2497.98	kJ/mol	Joback Method
hfus	63.16	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	9.193		Crippen Method
mcvol	418.560	ml/mol	McGowan Method
pc	638.66	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	951.71	K	Joback Method
tc	1184.03	K	Joback Method
tf	552.18	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1456.22	J/mol×K	951.71	Joback Method
cpg	1477.62	J/mol×K	990.43	Joback Method
cpg	1497.61	J/mol×K	1029.15	Joback Method
cpg	1516.34	J/mol×K	1067.87	Joback Method
cpg	1534.01	J/mol×K	1106.59	Joback Method
cpg	1550.79	J/mol×K	1145.31	Joback Method
cpg	1566.85	J/mol×K	1184.03	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=U368441&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